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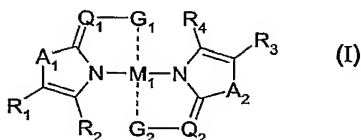
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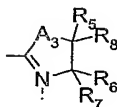
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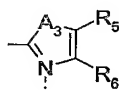
(54) Title: OPTICAL RECORDING MATERIALS HAVING HIGH STORAGE DENSITY



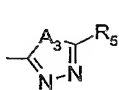
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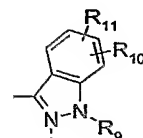
(IX)



(X)



(XI)



(XII)

(57) Abstract: The invention relates to an optical recording medium comprising a substrate, a reflecting layer and a recording layer based on compounds of formula (I) wherein G<sub>1</sub> and G<sub>2</sub> are each independently of the other, A<sub>1</sub> and A<sub>2</sub> are each independently of the other N(R<sub>12</sub>), O, S or Se and A<sub>3</sub> is C(C<sub>1</sub>-C<sub>5</sub>alkyl)<sub>2</sub>, C(C<sub>4</sub>-C<sub>5</sub> alkylene), N(R<sub>12</sub>), O, S, Se, N=C(R<sub>13</sub>) or unsubstituted or R<sub>14</sub>-substituted CH=CH; M<sub>1</sub> is a transition metal of groups (IX) to (XII), preferably Co, Cu, Ni, Pd or Zn, especially Co, Cu or Ni; Q<sub>1</sub> and Q<sub>2</sub> are each independently of the other C(R<sub>15</sub>), N or P... For the detailed definitions of the further substituents, see the description. Recording and playback are effected especially at a wavelength of from 350 to

500 nm, for example using a blue laser. The recording and playback quality is excellent and allows a high storage density. Also claimed are new compounds of formula (I), with the exception of the compounds disclosed in J. Org. Chem. 67/16, 5753-5772 [2002].

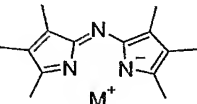
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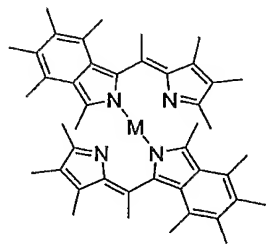
Optical recording materials having high storage density

The invention relates to new optical recording materials that have excellent recording and playback quality especially at a wavelength of 350-500 nm. Recording and playback can be effected very advantageously with high sensitivity at the same  
 5 wavelength, and the storage density that is achievable is significantly higher than in the case of known materials. In addition, the materials according to the invention have very good storage properties before and after recording, even under especially harsh conditions, such as exposure to sunlight or fluorescent lighting, heat and/or high humidity. In addition, their manufacture is simple and readily reproducible using  
 10 customary coating processes, such as spin-coating.

WO 02/082438 discloses the use of ionic salts, including those with metal complex anions, for optical recording materials. Those colorants are always substituted by alkyl, alkenyl, aryl or heteroaryl at the nitrogen atom. Their optical properties do not, however, fully satisfy increased demands. In particular, the refractive index as well  
 15 as the absorption and the steepness of the absorption band on its long wavelength flank in the solid still leave something to be desired.

JP-A-11/34500, JP-A-11/92479 and EP-A-0 903 733 disclose metal and boron

complexes of colorants of formulae  and



, which can be used at from 520 to 690 nm for optical

20 recording materials such as CD-R or DVD-R. Here too, however, the optical

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properties, especially the spectral properties in or near the UV range that are necessary for the highest possible storage densities, and the information density per unit surface area are not able to satisfy the highest demands as desired. The information density per unit surface area is far lower than is desirable.

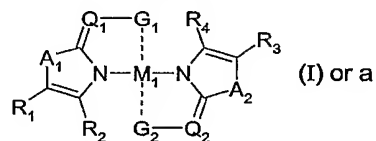
- 5 Conventional optical recording materials therefore satisfy high demands only to some extent, or do not satisfy all demands to an entirely satisfactory degree at the same time.

On the other hand, J. Org. Chem. 67/16, 5753-5772 [2002] describes the synthesis of a number of bis(o-azaheteroaryl)methanes and their coordination properties with respect to divalent transition metals, heteroaryl being 1,3-azol-2-yl, 1,3-benzazol-2-yl and azinyl and the transition metals being Zn, Cu, Co, Ni, Hg and Pd. *Inter alia* 2:1 salt complexes of bis(benzothiazol-2-yl)methane and bis(benzoxazol-2-yl)methane with copper(II) chloride and nickel(II) sulfate, and cobalt(II) chloride and palladium(II) nitrate are disclosed, whereas bis(thiazol-2-yl)methane yields, with  
 10  
 15 deprotonation, neutral 2:1 chelates with Zn(II), Cu(II), Ni(II) and Co(II). All substances are strongly coloured.

The aim of the invention is an optical recording medium having high information density, sensitivity and data reliability. Such a recording medium should be robust, durable and easy to use. Furthermore, it should be inexpensive to manufacture as a  
 20 mass-produced product and should require equipment that is as small and inexpensive as possible.

The invention therefore relates to an optical recording medium comprising a substrate, a recording layer and optionally one or more reflecting layers, wherein the

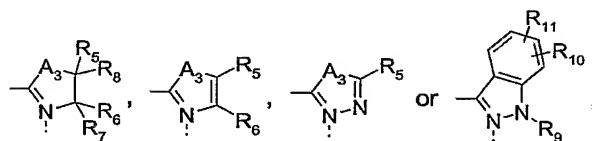
recording layer comprises a compound of formula



25 tautomer thereof, wherein

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G<sub>1</sub> and G<sub>2</sub> are each independently of the other



A<sub>1</sub> and A<sub>2</sub> are each independently of the other N(R<sub>12</sub>), O, S or Se and A<sub>3</sub> is C(C<sub>1</sub>-C<sub>5</sub>alkyl)<sub>2</sub>, C(C<sub>4</sub>-C<sub>5</sub>alkylene), N(R<sub>12</sub>), O, S, Se, N=C(R<sub>13</sub>) or unsubstituted or R<sub>14</sub>-substituted CH=CH;

M<sub>1</sub> is a transition metal of groups IX to XII, preferably Co, Cu, Ni, Pd or Zn, especially Co, Cu or Ni;

Q<sub>1</sub> and Q<sub>2</sub> are each independently of the other C(R<sub>15</sub>), N or P;

R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>, R<sub>4</sub>, R<sub>5</sub>, R<sub>6</sub>, R<sub>7</sub>, R<sub>8</sub> and R<sub>14</sub> are each independently of the others hydrogen, R<sub>18</sub>, or C<sub>6</sub>-C<sub>12</sub>aryl, C<sub>4</sub>-C<sub>12</sub>heteroaryl, C<sub>7</sub>-C<sub>12</sub>aralkyl or C<sub>5</sub>-C<sub>12</sub>heteroaralkyl each unsubstituted or substituted by one or more, where applicable identical or different, radicals R<sub>18</sub>; or

R<sub>1</sub> and R<sub>2</sub>, R<sub>3</sub> and R<sub>4</sub>, R<sub>5</sub> and R<sub>6</sub>, R<sub>5</sub> and R<sub>13</sub> and/or R<sub>5</sub> and R<sub>14</sub>, together in pairs, are C<sub>3</sub>-C<sub>6</sub>alkylene or C<sub>3</sub>-C<sub>6</sub>alkenylene, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R<sub>17</sub> and may be

uninterrupted or interrupted by O, S or N(R<sub>12</sub>), or 1,4-butadiene-1,3-dienylene,

or , each of which is unsubstituted or substituted by one or more, where

applicable identical or different, radicals R<sub>18</sub> and in which 1 or 2 carbon atoms may have been replaced by nitrogen;

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- $R_9$ ,  $R_{12}$  and  $R_{13}$  are each independently of the others  $C_1$ - $C_{24}$ alkyl,  $C_3$ - $C_{24}$ cycloalkyl,  $C_2$ - $C_{24}$ alkenyl,  $C_3$ - $C_{24}$ cycloalkenyl,  $C_1$ - $C_4$ alkyl-[O- $C_1$ - $C_4$ alkylene] $_m$  or  $C_1$ - $C_4$ alkyl-[NH- $C_1$ - $C_4$ alkylene] $_m$ , each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals  $R_{17}$ ; or  $C_6$ - $C_{12}$ aryl,  $C_4$ - $C_{12}$ heteroaryl,
- 5  $C_7$ - $C_{12}$ aralkyl or  $C_5$ - $C_{12}$ heteroaralkyl, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals  $R_{18}$ ;

- $R_{10}$ ,  $R_{11}$  and  $R_{18}$  are each independently of the others halogen, nitro, cyano, thiocyanato, hydroxy, O- $R_{19}$ , O-CO- $R_{19}$ , S- $R_{19}$ , CHO, COR $_{20}$ , CHOR $_{19}$ OR $_{23}$ , CR $_{20}$ OR $_{19}$ OR $_{23}$ ,  $R_{16}$ , N=N- $R_{16}$ , N=CR $_{19}$ R $_{20}$ , N=CR $_{21}$ R $_{22}$ , C( $R_{15}$ )=NR $_{19}$ ,
- 10 C( $R_{15}$ )=NR $_{21}$ , C( $R_{15}$ )=CR $_{21}$ R $_{22}$ , NH $_2$ , NH- $R_{19}$ , NR $_{19}$ R $_{20}$ , NH $_3^+$ , NH $_2$ R $_{19}^+$ , NHR $_{19}$ R $_{20}^+$ , NR $_{19}$ R $_{20}$ R $_{23}^+$ , CONH $_2$ , CONHR $_{19}$ , CONR $_{19}$ R $_{20}$ , SO $_2$ R $_{19}$ , SO $_2$ NH $_2$ , SO $_2$ NHR $_{19}$ , SO $_2$ NR $_{19}$ R $_{20}$ , COOH, COOR $_{19}$ , OCOOR $_{19}$ , NHCOR $_{19}$ , NR $_{19}$ COR $_{23}$ , NHCOOR $_{19}$ , NR $_{19}$ COOR $_{23}$ , ureido, NR $_{19}$ -CO-NHR $_{23}$ , B(OH) $_2$ , B(OH)(OR $_{19}$ ), B(OR $_{19}$ )OR $_{23}$ , phosphato, PR $_{19}$ R $_{23}$ , POR $_{19}$ OR $_{23}$ , P(=O)OR $_{19}$ OR $_{23}$ , OPR $_{19}$ R $_{23}$ , OPR $_{19}$ OR $_{23}$ ,
- 15 OP(=O)R $_{19}$ OR $_{23}$ , OP(=O)OR $_{19}$ OR $_{23}$ , OPO $_3$ R $_{19}$ , sulfato, sulfo, or  $C_1$ - $C_{12}$ alkyl,  $C_3$ - $C_{12}$ cycloalkyl,  $C_1$ - $C_{12}$ alkylthio,  $C_3$ - $C_{12}$ cycloalkylthio,  $C_1$ - $C_{12}$ alkoxy or  $C_3$ - $C_{12}$ cycloalkoxy each unsubstituted or substituted by one or more, where applicable identical or different, radicals  $R_{17}$ ;

- $R_{15}$  is hydrogen, cyano, hydroxy,  $C_1$ - $C_{12}$ alkoxy,  $C_3$ - $C_{12}$ cycloalkoxy,  $C_1$ - $C_{12}$ alkylthio,
- 20  $C_3$ - $C_{12}$ cycloalkylthio, amino, NHR $_{24}$ , NR $_{25}$ R $_{26}$ ,  $R_{27}$ , halogen, nitro, formyl, N=N- $R_{27}$ , C( $R_{14}$ )=CR $_{21}$ R $_{22}$ , C( $R_{14}$ )=NR $_{19}$ , COO- $R_{25}$ , carboxy, carbamoyl, CONH- $R_{25}$ , CONR $_{25}$ R $_{26}$ , N=CR $_{19}$ R $_{20}$ , or  $C_1$ - $C_{12}$ alkyl,  $C_3$ - $C_{12}$ cycloalkyl,  $C_2$ - $C_{12}$ alkenyl or  $C_3$ - $C_{12}$ cycloalkenyl each unsubstituted or substituted by one or more, where applicable identical or different, halogen, hydroxy,  $C_1$ - $C_{12}$ alkoxy or  $C_3$ - $C_{12}$ cycloalkoxy
- 25 radicals;

$R_{16}$  is  $C_6$ - $C_{12}$ aryl,  $C_4$ - $C_{12}$ heteroaryl,  $C_7$ - $C_{12}$ aralkyl or  $C_5$ - $C_{12}$ heteroaralkyl, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals  $R_{28}$ ;

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R<sub>17</sub> is halogen, hydroxy, O-R<sub>25</sub>, O-CO-R<sub>25</sub>, S-R<sub>25</sub>, NH<sub>2</sub>, NH-R<sub>25</sub>, NR<sub>25</sub>R<sub>26</sub>, NH<sub>3</sub><sup>+</sup>, NH<sub>2</sub>R<sub>25</sub><sup>+</sup>, NHR<sub>25</sub>R<sub>26</sub><sup>+</sup>, NR<sub>24</sub>R<sub>25</sub>R<sub>26</sub><sup>+</sup>, NR<sub>25</sub>-CO-R<sub>24</sub>, NR<sub>25</sub>COOR<sub>24</sub>, cyano, formyl, COO-R<sub>25</sub>, carboxy, carbamoyl, CONH-R<sub>25</sub>, CONR<sub>25</sub>R<sub>26</sub>, ureido, NH-CO-NHR<sub>24</sub>, NR<sub>25</sub>-CO-NHR<sub>24</sub>, phosphato, PR<sub>25</sub>R<sub>24</sub>, POR<sub>25</sub>OR<sub>24</sub>, P(=O)OR<sub>25</sub>OR<sub>24</sub>, OPR<sub>25</sub>R<sub>24</sub>,  
 5 OPR<sub>25</sub>OR<sub>24</sub>, OP(=O)R<sub>25</sub>OR<sub>24</sub>, OPO<sub>3</sub>R<sub>25</sub>, OP(=O)OR<sub>25</sub>OR<sub>24</sub>, SO<sub>2</sub>R<sub>25</sub>, sulfato, sulfo, R<sub>27</sub>, N=N-R<sub>27</sub>, or C<sub>1</sub>-C<sub>12</sub>alkoxy or C<sub>1</sub>-C<sub>12</sub>cycloalkoxy each unsubstituted or mono- or poly-substituted by halogen;

R<sub>19</sub>, R<sub>20</sub> and R<sub>23</sub> are each independently of the others R<sub>16</sub>, or C<sub>1</sub>-C<sub>12</sub>alkyl, C<sub>3</sub>-C<sub>12</sub>cycloalkyl, C<sub>2</sub>-C<sub>12</sub>alkenyl or C<sub>3</sub>-C<sub>12</sub>cycloalkenyl each unsubstituted or  
 10 substituted by one or more, where applicable identical or different, halogen, hydroxy, C<sub>1</sub>-C<sub>12</sub>alkoxy or C<sub>3</sub>-C<sub>12</sub>cycloalkoxy radicals; or

R<sub>14</sub> and R<sub>19</sub> together, R<sub>15</sub> and R<sub>19</sub> together and/or R<sub>19</sub> and R<sub>23</sub> together are C<sub>2</sub>-C<sub>12</sub>alkylene, C<sub>3</sub>-C<sub>12</sub>cycloalkylene, C<sub>2</sub>-C<sub>12</sub>alkenylene or C<sub>3</sub>-C<sub>12</sub>cycloalkenylene, each of which is unsubstituted or substituted by one or more, where applicable  
 15 identical or different, halogen, hydroxy, C<sub>1</sub>-C<sub>12</sub>alkoxy or C<sub>3</sub>-C<sub>12</sub>cycloalkoxy radicals; or

R<sub>19</sub> and R<sub>20</sub> together with the common nitrogen are pyrrolidine, piperidine, piperazine or morpholine, each of which is unsubstituted or mono- to tetra-substituted by C<sub>1</sub>-C<sub>4</sub>alkyl; or carbazole, phenoxazine or phenothiazine, each of which is unsub-  
 20 stituted or substituted by one or more, where applicable identical or different, radicals R<sub>28</sub>;

R<sub>21</sub> and R<sub>22</sub> are each independently of the other NR<sub>25</sub>R<sub>26</sub>, CN, CONH<sub>2</sub>, CONHR<sub>19</sub>, CONR<sub>19</sub>R<sub>20</sub> or COOR<sub>20</sub>;

R<sub>24</sub>, R<sub>25</sub> and R<sub>26</sub> are each independently of the others C<sub>1</sub>-C<sub>12</sub>alkyl, C<sub>3</sub>-C<sub>12</sub>cycloalkyl, C<sub>2</sub>-C<sub>12</sub>alkenyl, C<sub>3</sub>-C<sub>12</sub>cycloalkenyl, C<sub>6</sub>-C<sub>12</sub>aryl, C<sub>4</sub>-C<sub>12</sub>heteroaryl, C<sub>7</sub>-C<sub>12</sub>aralkyl or  
 25 C<sub>5</sub>-C<sub>12</sub>heteroaralkyl; or

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R<sub>25</sub> and R<sub>26</sub> together with the common nitrogen are pyrrolidine, piperidine, piperazine or morpholine, each of which is unsubstituted or mono- to tetra-substituted by C<sub>1</sub>-C<sub>4</sub>alkyl;

5 R<sub>27</sub> is C<sub>6</sub>-C<sub>12</sub>aryl, C<sub>4</sub>-C<sub>12</sub>heteroaryl, C<sub>7</sub>-C<sub>12</sub>aralkyl or C<sub>5</sub>-C<sub>12</sub>heteroaralkyl, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R<sub>18</sub>;

R<sub>28</sub> is nitro, SO<sub>2</sub>NHR<sub>25</sub>, SO<sub>2</sub>NR<sub>25</sub>R<sub>26</sub>, or C<sub>1</sub>-C<sub>12</sub>alkyl, C<sub>3</sub>-C<sub>12</sub>cycloalkyl, C<sub>1</sub>-C<sub>12</sub>alkylthio, C<sub>3</sub>-C<sub>12</sub>cycloalkylthio, C<sub>1</sub>-C<sub>12</sub>alkoxy or C<sub>3</sub>-C<sub>12</sub>cycloalkoxy each unsubstituted or substituted by one or more, where applicable identical or different, radicals R<sub>17</sub>; and

10 m is a number from 1 to 10.

When R<sub>5</sub> forms a bridge with R<sub>6</sub>, R<sub>5</sub> may not at the same time form a bridge with R<sub>13</sub> or R<sub>14</sub>.

It will be understood that acidic groups, such as carboxy, sulfo, sulfato and phosphato, may also be in the form of a salt, for example an alkali metal, alkaline  
 15 earth metal, ammonium or phosphonium salt, such as Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>, Mg<sup>2+</sup>, Ca<sup>2+</sup>, Cu<sup>2+</sup>, Ni<sup>2+</sup>, Fe<sup>2+</sup>, Co<sup>2+</sup>, Zn<sup>2+</sup>, Sn<sup>2+</sup>, La<sup>3+</sup>, ammonium, methylammonium, ethylammonium, isopropylammonium, <sup>TM</sup>Primene 81-R, <sup>TM</sup>Rosin Amine D, penta-decylammonium, <sup>TM</sup>Primene JM-T, dicyclohexylammonium, tetramethylammonium, tetraethylammonium, tetrabutylammonium, benzyltrimethylammonium, benzyl-  
 20 triethylammonium, methyltrioctylammonium, tridodecylmethylammonium, tetra-butylphosphonium, tetraphenylphosphonium, butyltriphenylphosphonium or ethyl-triphenylphosphonium, or any of the cations B-1 to B-169 mentioned in US-6 225 024, to which individually reference is expressly made here.

Halogen is chlorine, bromine, fluorine or iodine, preferably fluorine or chlorine,  
 25 especially fluorine on alkyl (for example trifluoromethyl,  $\alpha,\alpha,\alpha$ -trifluoroethyl or perfluorinated alkyl groups, such as heptafluoropropyl) and chlorine on aryl,

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heteroaryl or on the aryl moiety of aralkyl or on the heteroaryl moiety of hetero-aralkyl.

- Alkyl, cycloalkyl, alkenyl or cycloalkenyl can be straight-chain or branched, or monocyclic or polycyclic. Alkyl is, for example, methyl, straight-chain C<sub>2</sub>-C<sub>24</sub>alkyl or preferably branched C<sub>3</sub>-C<sub>24</sub>alkyl. Alkenyl is, for example, straight-chain C<sub>2</sub>-C<sub>20</sub>alkenyl or preferably branched C<sub>3</sub>-C<sub>24</sub>alkenyl. The invention therefore relates especially also to compounds of formula (I) containing branched C<sub>3</sub>-C<sub>24</sub>alkyl or branched C<sub>3</sub>-C<sub>24</sub>alkenyl, and also to optical recording materials comprising such compounds.
- C<sub>1</sub>-C<sub>24</sub>Alkyl is therefore, for example, methyl, ethyl, n-propyl, isopropyl, n-butyl, sec-butyl, isobutyl, tert-butyl, n-pentyl, 2-pentyl, 3-pentyl, 2,2-dimethylpropyl, n-hexyl, n-octyl, 1,1,3,3-tetramethylbutyl, 2-ethylhexyl, nonyl, decyl, dodecyl, tetradecyl, hexadecyl, octadecyl, eicosyl, heneicosyl, docosyl or tetracosyl. C<sub>3</sub>-C<sub>24</sub>Cycloalkyl is, for example, cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, trimethylcyclohexyl, menthyl, thujyl, bornyl, 1-adamantyl or 2-adamantyl.
- C<sub>2</sub>-C<sub>20</sub>Alkenyl and C<sub>3</sub>-C<sub>20</sub>cycloalkenyl are C<sub>2</sub>-C<sub>20</sub>alkyl and C<sub>3</sub>-C<sub>20</sub>cycloalkyl that is mono- or poly-unsaturated, wherein two or more double bonds may be isolated or conjugated, for example vinyl, allyl, 2-propen-2-yl, 2-buten-1-yl, 3-buten-1-yl, 1,3-butadien-2-yl, 2-cyclobuten-1-yl, 2-penten-1-yl, 3-penten-2-yl, 2-methyl-1-buten-3-yl, 2-methyl-3-buten-2-yl, 3-methyl-2-buten-1-yl, 1,4-pentadien-3-yl, 2-cyclopenten-1-yl, 2-cyclohexen-1-yl, 3-cyclohexen-1-yl, 2,4-cyclohexadien-1-yl, 1-*p*-menthen-8-yl, 4(10)-thujen-10-yl, 2-norbornen-1-yl, 2,5-norbornadien-1-yl, 7,7-dimethyl-2,4-norcaradien-3-yl or the various isomers of hexenyl, octenyl, nonenyl, decenyl, dodecenyl, tetradecenyl, hexadecenyl, octadecenyl, eicosenyl, heneicosenyl, docosenyl, tetracosenyl, hexadienyl, octadienyl, nonadienyl, decadienyl, dodecadienyl, tetradecadienyl, hexadecadienyl, octadecadienyl or eicosadienyl.

C<sub>7</sub>-C<sub>12</sub>Aralkyl is, for example, benzyl, 2-benzyl-2-propyl, β-phenyl-ethyl, 9-fluorenyl, α,α-dimethylbenzyl, ω-phenyl-butyl or ω-phenyl-hexyl. When C<sub>7</sub>-C<sub>12</sub>aralkyl is substituted, both the alkyl moiety and the aryl moiety of the aralkyl group can be



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substituted, the latter alternative being preferred.

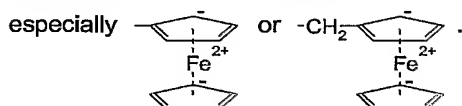
C<sub>6</sub>-C<sub>12</sub>Aryl is, for example, phenyl, naphthyl, biphenyl or 2-fluorenyl.

C<sub>4</sub>-C<sub>12</sub>Heteroaryl is an unsaturated or aromatic radical having 4n+2 conjugated  $\pi$ -electrons, for example 2-thienyl, 2-furyl, 2-pyridyl, 2-thiazolyl, 2-oxazolyl,

- 5 2-imidazolyl, isothiazolyl, triazolyl or any other ring system consisting of thiophene, furan, pyridine, thiazole, oxazole, imidazole, isothiazole, triazole, pyridine and benzene rings and unsubstituted or substituted by from 1 to 6 ethyl, methyl, ethylene and/or methylene substituents, for example benzotriazolyl, and in the case of N-heterocycles where applicable also those in the form of their N-oxides.

- 10 C<sub>5</sub>-C<sub>12</sub>Heteroaralkyl is, for example, C<sub>1</sub>-C<sub>8</sub>alkyl substituted by C<sub>4</sub>-C<sub>11</sub>heteroaryl.

Furthermore, aryl and aralkyl can also be aromatic groups bonded to a metal, for example in the form of metallocenes of transition metals known *per se*, more



- The transition metal M<sub>1</sub> is preferably in the form of a doubly positively charged cation, for example Co<sup>2+</sup>, Cu<sup>2+</sup>, Ni<sup>2+</sup>, Pd<sup>2+</sup> or Zn<sup>2+</sup>, especially Co<sup>2+</sup>, Cu<sup>2+</sup> or Ni<sup>2+</sup>.

- The compound of formula (I) may also be a cation which has been neutralised with an inorganic, organic or organometallic anion, for example when one or more ammonium groups are present or when the transition metal has one or more excess positive charges, such as in Co<sup>3+</sup>. The inorganic, organic or organometallic anion
- 20 may be, for example, the anion of a mineral acid, of the conjugated base of an organic acid (for example an alcoholate, phenolate, carboxylate, sulfonate or phosphonate) or an organometallic complex anion, for example fluoride, chloride, bromide, iodide, perchlorate, periodate, nitrate, hydrogen carbonate, ½ carbonate, ½ sulfate, C<sub>1</sub>-C<sub>4</sub>alkyl sulfate, hydrogen sulfate, ⅓ phosphate, ½ hydrogen phos-

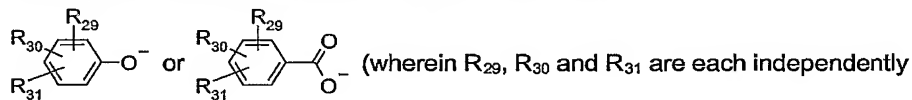
- 9 -

- phate, dihydrogen phosphate,  $\frac{1}{2}$  C<sub>1</sub>-C<sub>4</sub>alkanephosphonate, C<sub>1</sub>-C<sub>4</sub>alkane-C<sub>1</sub>-C<sub>12</sub>alkylphosphonate, di-C<sub>1</sub>-C<sub>4</sub>alkylphosphinate, tetrafluoroborate, hexafluorophosphate, hexafluoroantimonate, acetate, trifluoroacetate, heptafluorobutyrate,  $\frac{1}{2}$  oxalate, methanesulfonate, trifluoromethanesulfonate, benzenesulfonate, tosylate,
- 5 p-chlorobenzenesulfonate, p-nitrobenzenesulfonate, phenolate, benzoate or a negatively charged metal complex.

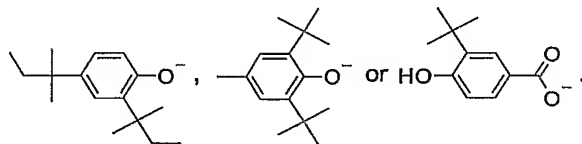
The person skilled in the art will readily recognise that it is also possible to use other anions with which he is familiar. It will be self-evident to him that  $\frac{1}{x}$  of an inorganic, organic or organometallic anion having x negative charges, for example  $\frac{1}{2} \cdot \text{SO}_4^{2-}$ , is

10 a multiply charged anion which neutralises several singly charged cations or a cation having x charges, as the case may be.

Phenolates or carboxylates are, for example, of formula



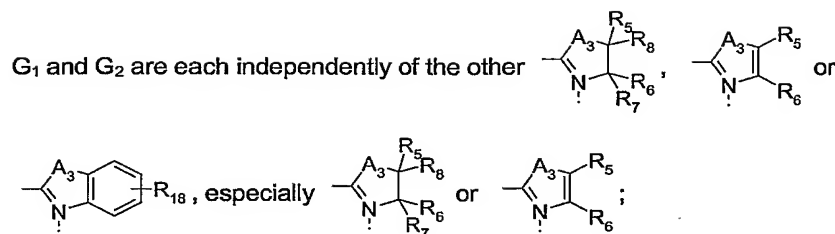
- of the others hydrogen, R<sub>18</sub>, or C<sub>6</sub>-C<sub>12</sub>aryl, C<sub>4</sub>-C<sub>12</sub>heteroaryl, C<sub>7</sub>-C<sub>12</sub>aralkyl or
- 15 C<sub>5</sub>-C<sub>12</sub>heteroaralkyl each unsubstituted or substituted by one or more, where applicable identical or different, radicals R<sub>18</sub>, for example anions of C<sub>1</sub>-C<sub>12</sub>alkylated, especially tert-C<sub>4</sub>-C<sub>8</sub>alkylated, phenols and benzoic acids, such as



Preference is given to compounds of formula (I) wherein

- 20 A<sub>1</sub>, A<sub>2</sub> and A<sub>3</sub> are each independently of the others O, S or N(R<sub>12</sub>) and/or Q<sub>1</sub> and Q<sub>2</sub> are C(R<sub>15</sub>) or N;

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R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>, R<sub>4</sub>, R<sub>5</sub>, R<sub>6</sub>, R<sub>7</sub>, R<sub>8</sub> and R<sub>14</sub> are each independently of the others hydrogen, R<sub>18</sub>, or C<sub>6</sub>-C<sub>12</sub>aryl or C<sub>7</sub>-C<sub>12</sub>aralkyl each unsubstituted or substituted by one or more, where applicable identical or different, radicals R<sub>16</sub>;

R<sub>9</sub>, R<sub>12</sub> and R<sub>13</sub> are each independently of the others unsubstituted or R<sub>17</sub>-substituted C<sub>1</sub>-C<sub>8</sub>alkyl;

R<sub>10</sub> and R<sub>18</sub> are each independently of the other halogen, nitro, cyano, O-R<sub>19</sub>, formyl, CH=C(CN)<sub>2</sub>, CH=C(CN)CONH<sub>2</sub>, CH=C(CN)CONHR<sub>19</sub>, CH=C(CN)CONR<sub>19</sub>R<sub>20</sub>, CH=C(CN)COOR<sub>19</sub>, CH=C(COOR<sub>19</sub>)COOR<sub>20</sub>, CONH<sub>2</sub>, CONHR<sub>19</sub>, CONR<sub>19</sub>R<sub>20</sub>, SO<sub>2</sub>C<sub>1</sub>-C<sub>12</sub>alkyl, SO<sub>2</sub>NH<sub>2</sub>, SO<sub>2</sub>NHR<sub>19</sub>, SO<sub>2</sub>NR<sub>19</sub>R<sub>20</sub>, COOH, COOR<sub>19</sub>, NHCOR<sub>19</sub>, NR<sub>19</sub>COR<sub>23</sub>, NHCOOR<sub>19</sub>, NR<sub>19</sub>COOR<sub>23</sub>, ureido, P(=O)OR<sub>19</sub>OR<sub>23</sub>, sulfo, or C<sub>1</sub>-C<sub>12</sub>alkyl, C<sub>1</sub>-C<sub>12</sub>alkylthio or C<sub>1</sub>-C<sub>12</sub>alkoxy each unsubstituted or substituted by one or more, where applicable identical or different, radicals R<sub>17</sub>;

R<sub>15</sub> is hydrogen, cyano, halogen, nitro, formyl, N=N-R<sub>27</sub>, C(R<sub>14</sub>)=CR<sub>21</sub>R<sub>22</sub>, C(R<sub>14</sub>)=NR<sub>19</sub>, COO-R<sub>25</sub>, carboxy, carbamoyl, CONH-R<sub>25</sub>, CONR<sub>25</sub>R<sub>26</sub>, or C<sub>1</sub>-C<sub>12</sub>alkyl unsubstituted or substituted by one or more halogen substituents;

R<sub>16</sub> is unsubstituted or substituted C<sub>6</sub>-C<sub>12</sub>aryl or C<sub>7</sub>-C<sub>12</sub>aralkyl, especially a metallocenyl radical;

R<sub>17</sub> is halogen, hydroxy, O-R<sub>25</sub>, amino, NH-R<sub>25</sub>, NR<sub>25</sub>R<sub>26</sub>, NR<sub>25</sub>-CO-R<sub>24</sub>, NR<sub>25</sub>COOR<sub>24</sub>, cyano, COO-R<sub>25</sub>, carboxy, CONH-R<sub>25</sub>, CONR<sub>25</sub>R<sub>26</sub>, sulfato, sulfo, or C<sub>1</sub>-C<sub>12</sub>alkoxy unsubstituted or mono- or poly-substituted by halogen;

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R<sub>19</sub>, R<sub>20</sub> and R<sub>23</sub> are each independently of the others C<sub>1</sub>-C<sub>12</sub>alkyl unsubstituted or substituted by one or more, where applicable identical or different, halogen, hydroxy or C<sub>1</sub>-C<sub>12</sub>alkoxy radicals, or unsubstituted C<sub>6</sub>-C<sub>12</sub>aryl or C<sub>7</sub>-C<sub>12</sub>aralkyl; or

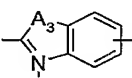
R<sub>19</sub> and R<sub>20</sub> together with the common nitrogen are morpholine, or piperidine N-substituted by C<sub>1</sub>-C<sub>4</sub>alkyl;

R<sub>25</sub>, R<sub>26</sub> and R<sub>24</sub> are each independently of the others C<sub>1</sub>-C<sub>12</sub>alkyl, C<sub>2</sub>-C<sub>12</sub>alkenyl, C<sub>6</sub>-C<sub>12</sub>aryl or C<sub>7</sub>-C<sub>12</sub>aralkyl; or

R<sub>25</sub> and R<sub>26</sub> together with the common nitrogen are morpholine, or piperidine N-substituted by C<sub>1</sub>-C<sub>4</sub>alkyl; and/or

m is a number from 1 to 4.

Special preference is given to compounds of formula (I) wherein Q<sub>1</sub> and Q<sub>2</sub> are

C(R<sub>15</sub>); G<sub>1</sub> and G<sub>2</sub> are ; and A<sub>1</sub>, A<sub>2</sub> and A<sub>3</sub> are O, S or N(R<sub>12</sub>);

R<sub>12</sub> is C<sub>1</sub>-C<sub>24</sub>alkyl, C<sub>1</sub>-C<sub>4</sub>alkyl-[O-C<sub>1</sub>-C<sub>4</sub>alkylene]<sub>m</sub> or C<sub>1</sub>-C<sub>4</sub>alkyl-[NH-C<sub>1</sub>-C<sub>4</sub>alkylene]<sub>m</sub>, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R<sub>17</sub>, or C<sub>6</sub>-C<sub>12</sub>aryl unsubstituted or substituted by one or more, where applicable identical or different, radicals R<sub>18</sub>;

R<sub>15</sub> is hydrogen, cyano, COO-R<sub>25</sub> or C<sub>1</sub>-C<sub>12</sub>alkyl;

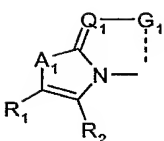
R<sub>17</sub> is halogen, hydroxy, O-R<sub>25</sub>, cyano, COO-R<sub>25</sub> or carboxy; and

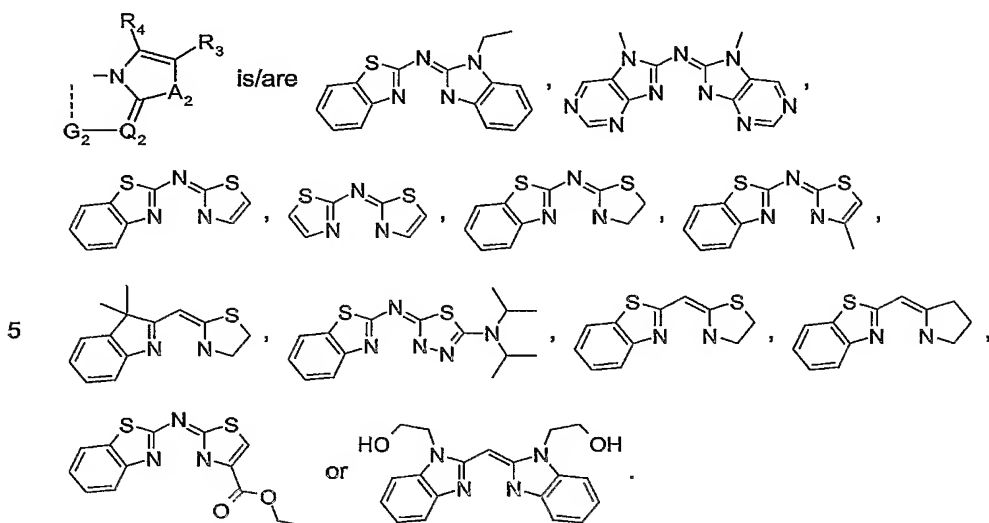
R<sub>18</sub> is halogen, nitro, cyano, O-R<sub>19</sub>, CH=C(CN)<sub>2</sub>, COOR<sub>19</sub>, ureido, CONR<sub>25</sub>R<sub>26</sub>, SO<sub>2</sub>R<sub>25</sub>, P(=O)OR<sub>19</sub>OR<sub>23</sub> or unsubstituted or substituted C<sub>1</sub>-C<sub>12</sub>alkyl.

Those preferred meanings apply both individually and in any combination. The compounds of formula (I) generally exhibit more advantageous properties, the more

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preferred individual features they have.

Also preferred are compounds of formula (I) wherein  and/or



The recording layer advantageously comprises a compound of formula (I) or a mixture of such compounds as main component, for example at least 30 % by weight, preferably at least 60 % by weight, especially at least 80 % by weight.

- 10 Further customary constituents are possible, for example other chromophores (for example those disclosed in WO 01/75873, or others having an absorption maximum at from 300 to 1000 nm), stabilisers,  $^1\text{O}_2$ -, triplet- or luminescence-quenchers, melting-point reducers, decomposition accelerators or any other additives that have
- 15 fluorescence-quenchers are added if desired.

When the recording layer comprises further chromophores, the amount of such

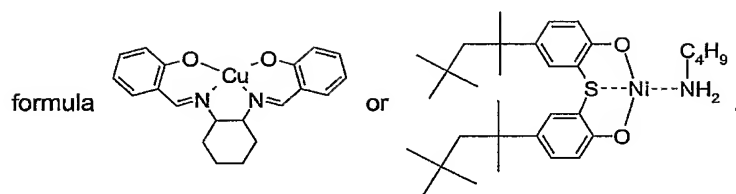
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chromophores should preferably be small, so that the absorption thereof at the wavelength of the inversion point of the longest-wavelength flank of the absorption of the entire solid layer is a fraction of the absorption of the pure compound of formula (I) in the entire solid layer at the same wavelength, advantageously at most  $\frac{1}{3}$ ,  
5 preferably at most  $\frac{1}{5}$ , especially at most  $\frac{1}{10}$ . The absorption maximum is preferably higher than 425 nm, especially higher than 500 nm.

Stabilisers,  $^1\text{O}_2$ -, triplet- or luminescence-quenchers are, for example, metal complexes of N- or S-containing enolates, phenolates, bisphenolates, thiolates or bithiolates or of azo, azomethine or formazan dyes, such as bis(4-dimethylamino-  
10 dithiobenzil)nickel [CAS N° 38465-55-3], <sup>®</sup>Irgalan Bordeaux EL, <sup>®</sup>Cibafast N or similar compounds, hindered phenols and derivatives thereof (optionally also as counter-ions X), such as <sup>®</sup>Cibafast AO, o-hydroxyphenyl-triazoles or -triazines or other UV absorbers, such as <sup>®</sup>Cibafast W or <sup>®</sup>Cibafast P or hindered amines (TEMPO or HALS, also as nitroxides or NOR-HALS, optionally also as counter-ions  
15 X), and also as cations diimmonium, Paraquat<sup>™</sup> or Orthoquat<sup>™</sup> salts, such as <sup>®</sup>Kayasorb IRG 022, <sup>®</sup>Kayasorb IRG 040, optionally also as radical ions, such as N,N,N',N'-tetrakis(4-dibutylaminophenyl)-p-phenyleneamine-ammonium hexafluorophosphate, hexafluoroantimonate or perchlorate. The latter are available from Organica (Wolfen / DE); <sup>®</sup>Kayasorb brands are available from Nippon Kayaku Co.  
20 Ltd., and <sup>®</sup>Irgalan and <sup>®</sup>Cibafast brands are available from Ciba Spezialitätenchemie AG.

Many such structures are known, some of them also in connection with optical recording media, for example from US-5 219 707, JP-A-06/199045, JP-A-07/76169, JP-A-07/262604 or JP-A-2000/272241. They may be, for example, salts of the metal  
25 complex anions disclosed above with any desired cations, for example the cations disclosed above, or metal complexes, illustrated, for example, by a compound of

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The person skilled in the art will know from other optical information media, or will easily identify, which additives in which concentration are particularly well suited to which purpose. Suitable concentrations of additives are, for example, from 0.001 to  
 5 1000% by weight, preferably from 1 to 50% by weight, based on the recording medium of formula (I).

- The optical recording materials according to the invention exhibit excellent spectral properties of the solid amorphous recording layer. The refractive index is extraordinarily high, in some cases even above 2.5. By virtue of an aggregation  
 10 tendency in the solid that is surprisingly low for such compounds, the absorption band is narrow and intense, the absorption band being especially steep on the long-wavelength side. Crystallites are unexpectedly and very advantageously not formed or are formed only to a negligible extent. The reflectivity of the layers in the range of the writing and reading wavelength is very high in the unwritten state.
- 15 By virtue of those excellent layer properties it is possible to obtain a rapid optical recording having high sensitivity, high reproducibility and geometrically very precise mark boundaries, the refractive index and the reflectivity changing substantially, which gives a high degree of contrast. The differences in the mark lengths and the interval distances ("jitter") are very small, which enables a high storage density to be  
 20 obtained using a relatively thin recording channel with a narrow track spacing ("pitch"). In addition, the recorded data are played back with an astonishingly low error rate, so that error correction requires only a small amount of storage space.

By virtue of the excellent solubility, including in apolar solvents, solutions can be

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used even in high concentrations without troublesome precipitation, for example during storage, so that problems during spin-coating are largely eliminated. This applies especially to compounds containing branched C<sub>3</sub>-C<sub>8</sub>alkyl.

Recording and playback can take place at the same wavelength, therefore  
5 advantageously requiring a simple optical system with a single laser source of advantageously from 350 to 500 nm, preferably from 370 to 450 nm. Especially preferred is the UV range from 370 to 390 nm, especially approximately 380 nm, or especially at the edge of the visible range of from 390 to 430 nm, more especially approximately 405 ± 5 nm. In the field of compact, blue or violet laser diodes (such  
10 as Nichia GaN 405 nm) with an optical system of high numerical aperture the marks can be so small and the tracks so narrow that up to about 20 to 25 Gb per recording layer is achievable on a 120 mm disc. At 380 nm it is possible to use indium-doped UV-VCSELs (Vertical-Cavity Surface-Emitting Laser), which laser source already exists as a prototype [Jung Han *et al.*, see MRS Internet J. Nitride Semicond. Res.  
15 5S1, W6.2 (2000)].

The invention therefore relates also to a method of recording or playing back data, wherein the data on an optical recording medium according to the invention are recorded or played back at a wavelength of from 350 to 500 nm.

The recording medium is based on the structure of known recording media and is,  
20 for example, analogous to those mentioned above. It may be composed, for example, of a transparent substrate, a recording layer comprising at least one of the compounds of formula (I), a reflector layer and a covering layer, the writing and readout being effected through the substrate.

Suitable substrates are, for example, glass, minerals, ceramics and thermosetting  
25 and thermoplastic plastics. Preferred supports are glass and homo- or co-polymeric plastics. Suitable plastics are, for example, thermoplastic polycarbonates, polyamides, polyesters, polyacrylates and polymethacrylates, polyurethanes, polyolefins, polyvinyl chloride, polyvinylidene fluoride, polyimides, thermosetting polyesters and



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epoxy resins. Special preference is given to polycarbonate substrates which can be produced, for example, by injection-moulding. The substrate can be in pure form or may comprise customary additives, for example UV absorbers or dyes, as proposed e.g. in JP-A-04/167239 as light stabilisation for the recording layer. In the latter case  
5 it may be that in the range of the writing wavelength (emission wavelength of the laser) the dye added to the support substrate has no or at most only very low absorption, preferably up to a maximum of about 20% of the laser light focussed onto the recording layer.

The substrate is advantageously transparent over at least a portion of the range  
10 from 350 to 500 nm, so that it is permeable to, for example, at least 80 % of the incident light of the writing or readout wavelength. The substrate is advantageously from 10  $\mu\text{m}$  to 2 mm thick, preferably from 100 to 1200  $\mu\text{m}$  thick, especially from 600 to 1100  $\mu\text{m}$  thick, with a preferably spiral guide groove (track) on the coating side, a groove depth of from 10 to 200 nm, preferably from 80 to 150 nm, a groove width of  
15 from 100 to 400 nm, preferably from 150 to 250 nm, and a spacing between two turns of from 200 to 600 nm, preferably from 350 to 450 nm. Grooves of different cross-sectional shape are known, for example rectangular, trapezoidal or V-shaped. Analogously to the known CD-R and DVD-R media, the guide groove may additionally undergo a small periodic or quasi-periodic lateral deflection (wobble), so  
20 that synchronisation of the speed of rotation and the absolute positioning of the reading head (pick-up) are made possible. Instead of, or in addition to, the deflection, the same function can be performed by markings between adjacent grooves (pre-pits).

The recording medium is applied, for example, by application of a solution by spin-coating, the objective being to produce a layer that is as amorphous as possible, the  
25 thickness of which layer is advantageously from 0 to 40 nm, preferably from 1 to 20 nm, especially from 2 to 10 nm, on the surface ("land") and, depending upon the geometry of the groove, advantageously from 20 to 150 nm, preferably from 50 to 120 nm, especially from 60 to 100 nm, in the groove.

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Reflecting materials suitable for the reflector layer include especially metals, which provide good reflection of the laser radiation used for recording and playback, for example the metals of Main Groups III, IV and V and of the Sub-Groups of the Periodic Table of the Elements. Al, In, Sn, Pb, Sb, Bi, Cu, Ag, Au, Zn, Cd, Hg, Sc, Y,  
5 La, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Fe, Co, Ni, Ru, Rh, Pd, Os, Ir, Pt and the lanthanide metals Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu and alloys thereof are especially suitable. On account of its high reflectivity and ease of production special preference is given to a reflective layer of aluminium, silver, gold or an alloy thereof (for example a white gold alloy), especially aluminium on  
10 economic and ecological grounds. The reflector layer is advantageously from 5 to 200 nm thick, preferably from 10 to 100 nm thick, especially from 40 to 60 nm thick, but reflector layers of greater thickness, for example 1 mm thick or even more, are also possible.

Materials suitable for the covering layer include chiefly plastics, which are applied in  
15 a thin layer to the reflector layer either directly or with the aid of adhesion promoters. It is advantageous to select mechanically and thermally stable plastics having good surface properties, which can be modified further, for example written on. The plastics may be thermosetting plastics and thermoplastic plastics. Directly applied covering layers are preferably radiation-cured (e.g. using UV radiation) coatings,  
20 which are particularly simple and economical to produce. A wide variety of radiation-curable materials are known. Examples of radiation-curable monomers and oligomers are acrylates and methacrylates of diols, triols and tetrols, polyimides of aromatic tetracarboxylic acids and aromatic diamines having C<sub>1</sub>-C<sub>4</sub>alkyl groups in at least two ortho-positions of the amino groups, and oligomers with dialkylmaleinimidyl  
25 groups, e.g. dimethylmaleinimidyl groups. For covering layers that are applied using adhesion promoters it is preferable to use the same materials as those used for the substrate layer, especially polycarbonates. The adhesion promoters used are preferably likewise radiation-curable monomers and oligomers. Instead of the covering layer applied using an adhesion promoter there may also be used a second  
30 substrate comprising a recording and reflector layer, so that the recording medium is

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playable on both sides. Preference is given to a symmetrical structure, the two parts being joined together at the reflector side by an adhesion promoter directly or by way of an intermediate layer.

In such a structure, the optical properties of the covering layer, or the covering materials, are essentially unimportant *per se* provided that, where applicable, curing thereof e.g. by UV radiation is achieved. The function of the covering layer is to ensure the mechanical strength of the recording medium as a whole and, if necessary, the mechanical strength of thin reflector layers. If the recording medium is sufficiently robust, for example when a thick reflector layer is present, it is even possible to dispense with the covering layer altogether. The thickness of the covering layer depends upon the thickness of the recording medium as a whole, which should preferably be a maximum of about 2 mm thick. The covering layer is preferably from 10  $\mu\text{m}$  to 1 mm thick.

The recording media according to the invention may also have additional layers, for example interference layers or barrier layers. It is also possible to construct recording media having a plurality of (for example from two to ten) recording layers. The structure and the use of such materials are known to the person skilled in the art. Where present, interference layers are preferably arranged between the recording layer and the reflecting layer and/or between the recording layer and the substrate and consist of a dielectric material, for example as described in EP-A-0 353 393 of  $\text{TiO}_2$ ,  $\text{Si}_3\text{N}_4$ ,  $\text{ZnS}$  or silicone resins.

The recording media according to the invention can be produced by processes known *per se*, it being possible for various methods of coating to be employed depending upon the materials used and their function.

Suitable coating methods are, for example, immersion, pouring, brush-coating, blade-application and spin-coating, as well as vapour-deposition methods carried out under a high vacuum. When, for example, pouring methods are used, solutions in organic solvents are generally employed. When solvents are employed, care should

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be taken that the supports used are insensitive to those solvents. Suitable coating methods and solvents are described, for example, in EP-A-0 401 791.

The recording layer is applied preferably by the application of a dye solution by spin-coating, solvents that have proved satisfactory being especially alcohols, e.g.

5 2-methoxyethanol, isopropanol or n-butanol, hydroxyketones, for example diacetone alcohol or 3-hydroxy-3-methyl-2-butanone, hydroxy esters, for example lactic acid methyl ester or isobutyric acid methyl ester, or preferably fluorinated alcohols, for example 2,2,2-trifluoroethanol or 2,2,3,3-tetrafluoro-1-propanol, and mixtures thereof. Further suitable solvents are disclosed, for example, in EP-A-0 483 387.

10 The application of the metallic reflector layer is preferably effected by sputtering or by vapour-deposition *in vacuo*. Such techniques are known and are described in specialist literature (e.g. J.L. Vossen and W. Kern, "Thin Film Processes", Academic Press, 1978). The operation can advantageously be carried out continuously and achieves good reflectivity and a high degree of adhesiveness of the metallic reflector  
15 layer.

Recording is carried out in accordance with known methods by writing pits (marks) of fixed or variable length by means of a modulated, focussed laser beam guided at a constant or variable speed over the surface of the recording layer. Readout of information is carried out according to methods known *per se* by registering the  
20 change in reflection using laser radiation, for example as described in "CD-Player und R-DAT Recorder" (Claus Biaesch-Wiepeke, Vogel Buchverlag, Würzburg 1992). The person skilled in the art will be familiar with the requirements.

The information-containing medium according to the invention is especially an optical information material of the WORM type. It can be used, for example, analogously to  
25 CD-R (compact disc - recordable) or DVD-R (digital video disc - recordable) in computers, and also as storage material for identification and security cards or for the production of diffractive optical elements, for example holograms.

- 20 -

Alternatively, however, there are also recording media which differ substantially from CD-R and DVD-R and in which recording and playback take place not through the substrate but through the covering layer ("in-groove recording"). Accordingly the respective roles of the covering layer and the substrate, especially the geometry and the optical properties, are reversed in comparison with the structure described above. Analogous concepts are described a number of times in Proceedings SPIE-Int. Soc. Opt. Eng. 1999, 3864 for digital video recordings in conjunction with a blue GaN laser diode. For such recording media, which are especially suitable for a high storage density and have correspondingly small marks ("pits"), precise focussing is important, so that the manufacturing process, while essentially analogous, is considerably more awkward.

The compounds of formula (I) according to the invention, however, also meet the increased demands of an inverse layer structure surprisingly well. Preference is therefore given to an inverse layer structure having the layer sequence substrate, reflector layer, recording layer and covering layer. The recording layer is therefore located between the reflector layer and the covering layer. A thin covering layer approximately from 50 to 400  $\mu\text{m}$  in thickness is especially advantageous (typically 100  $\mu\text{m}$  at a numerical aperture of 0.85).

The recording and reflector layers in an inverse layer structure have in principle the same functions as indicated above. As with the groove geometry, they therefore usually have dimensions within the ranges indicated above.

The inverse layer structure requires particularly high standards, which the compounds used according to the invention fulfil astonishingly well, for example when the recording layer is applied to the metallic reflector layer and especially when a covering layer is applied to the recording layer, the covering layer being required to provide the recording layer with adequate protection against rubbing, photo-oxidation, fingerprints, moisture and other environmental effects and advantageously having a thickness in the range of from 0.01 to 0.5 mm, preferably in the range of

- 21 -

from 0.05 to 0.2 mm, especially in the range of from 0.08 to 0.13 mm.

The covering layer preferably consists of a material that exhibits a transmission of 80% or above at the writing or readout wavelength of the laser. Suitable materials for the covering layer include, for example, those materials mentioned above, but  
5 especially polycarbonate (such as Pure Ace<sup>®</sup> or Panlite<sup>®</sup>, Teijin Ltd), cellulose triacetate (such as Fujitac<sup>®</sup>, Fuji Photo Film) or polyethylene terephthalate (such as Lumirror<sup>®</sup>, Toray Industry), special preference being given to polycarbonate. Especially in the case of directly applied covering layers, radiation-cured coatings, such as those already described above, are advantageous, for example SD 347<sup>™</sup>  
10 (Dainippon Ink).

The covering layer can be applied directly to the solid recording layer by means of a suitable adhesion promoter. In another embodiment, there is applied to the solid recording layer an additional, thin separating layer of a metallic, crosslinked organo-metallic or preferably dielectric inorganic material, for example in a thickness of from  
15 0.001 to 10  $\mu\text{m}$ , preferably from 0.005 to 1  $\mu\text{m}$ , especially from 0.01 to 0.1  $\mu\text{m}$ , for example from 0.05 to 0.08  $\mu\text{m}$  in the case of dielectric separating layers and from 0.01 to 0.03  $\mu\text{m}$  in the case of metallic separating layers. Separating layers and corresponding methods are disclosed in WO 02/082438, to which reference is expressly made here. If desired, such coatings can be applied, for example, in the  
20 same thickness also between the support material and the metallic reflector layer or between the metallic reflector layer and the optical recording layer. This may be advantageous in certain cases, for example when a silver reflector is used in combination with sulfur-containing additives in the recording layer.

In a special variant, there is applied to the solid recording layer an additional, thin  
25 separating layer of a metallic, crosslinked organometallic or dielectric inorganic material, for example in a thickness of from 0.001 to 10  $\mu\text{m}$ , preferably from 0.005 to 1  $\mu\text{m}$ , especially from 0.01 to 0.1  $\mu\text{m}$ . On account of their high reflectivity, metallic separating layers should advantageously be a maximum of 0.03  $\mu\text{m}$  thick.

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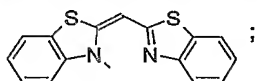
Separating layers and corresponding methods are disclosed in WO 02/082438, to which reference is expressly made here.

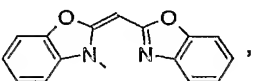
Some of the compounds used according to the invention are known, especially from J. Org. Chem. 67/16, 5753-5772 [2002].

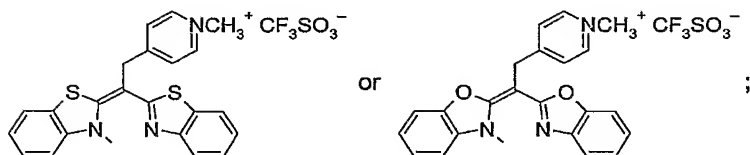
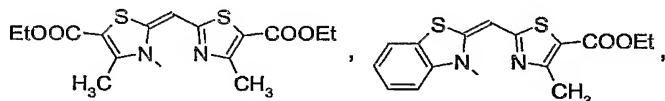
- 5 It is also possible, however, to prepare analogously to the known compounds new compounds that can be used in accordance with the invention in optical recording media.

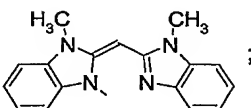
The invention therefore relates also to compounds of formula (I), with the exception of the already known compounds of formula  $M_2(Z_1)_2$ , wherein:

- 10 •  $M_2$  is Co(II), Cu(II), Hg(II), Ni(II), Pd(II) or Zn(II) and  $Z_1$  is

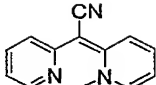


- $M_2$  is Co(II), Cu(II), Ni(II), Pd(II) or Zn(II) and  $Z_1$  is  ,

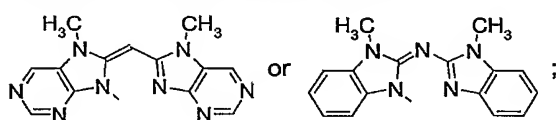


- 15 •  $M_2$  is Co(II), Cu(II), Ni(II) or Zn(II) and  $Z_1$  is  ;

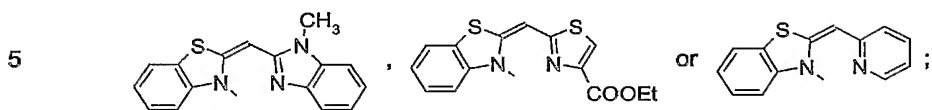
- 23 -

- $M_2$  is Cu(II), Pd(II) or Zn(II) and  $Z_1$  is  ;

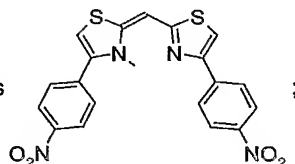
- $M_2$  is Co(II), Cu(II) or Zn(II) and  $Z_1$  is



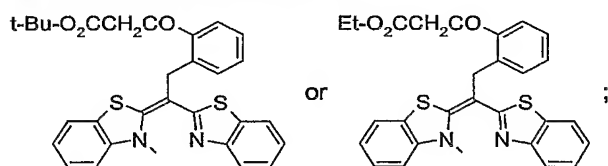
- $M_2$  is Cu(II) or Zn(II) and  $Z_1$  is



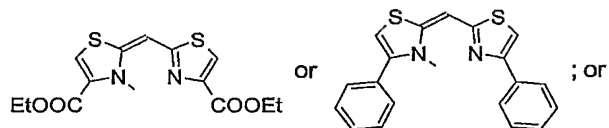
- $M_2$  is Co(II) or Cu(II) and  $Z_1$  is



- $M_2$  is Pd(II) or Zn(II) and  $Z_1$  is

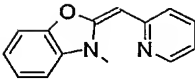
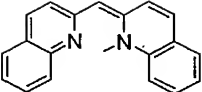


- $M_2$  is Cu(II) and  $Z_1$  is

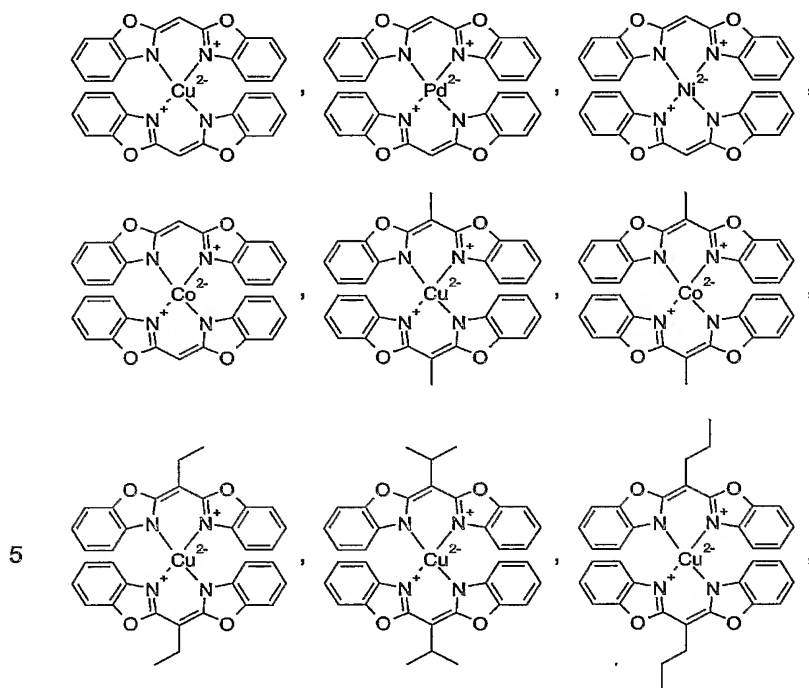




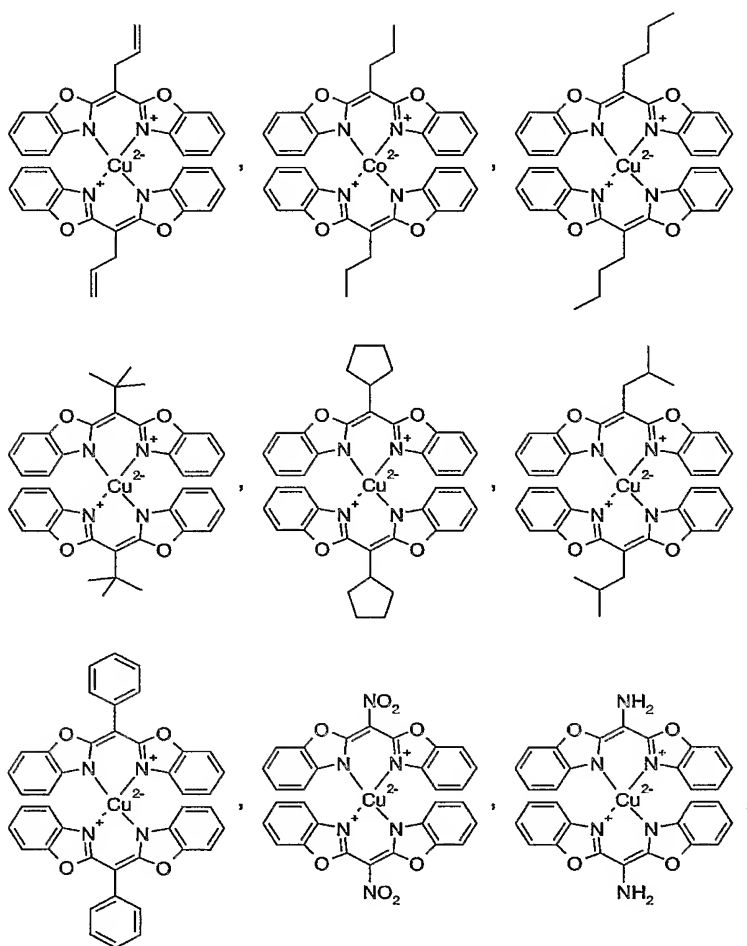
- 24 -

- $M_2$  is Zn(II) and  $Z_1$  is  or .

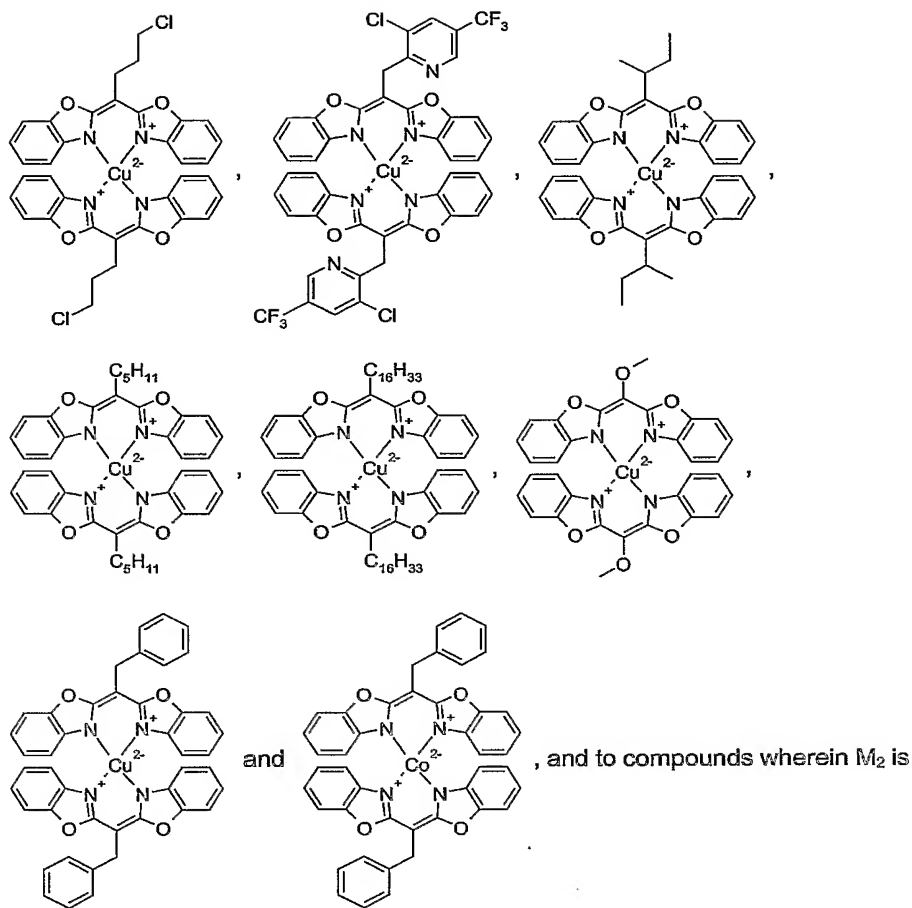
Reference is made especially to compounds of formulae



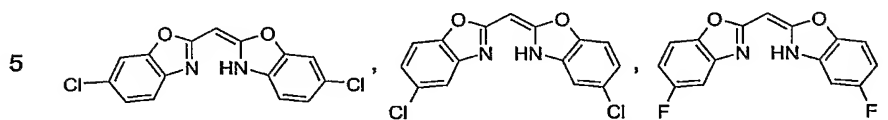
- 25 -



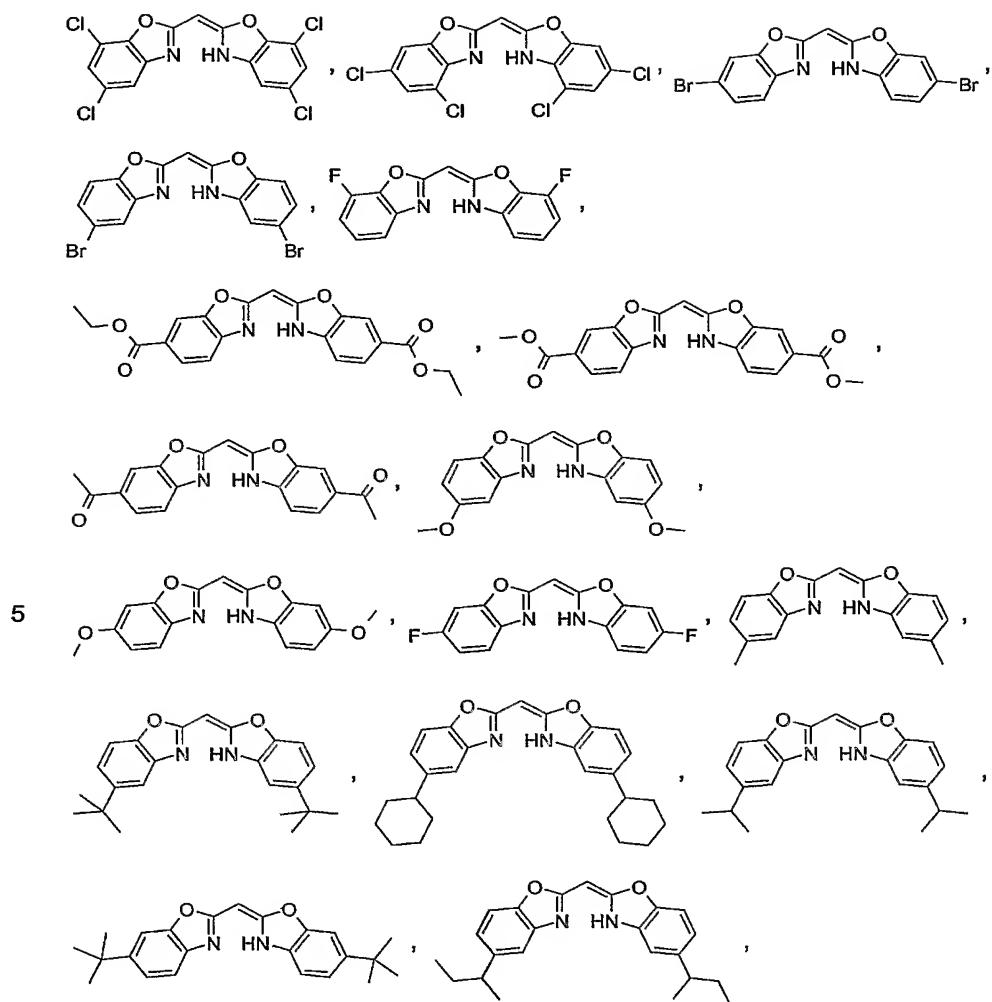
- 26 -

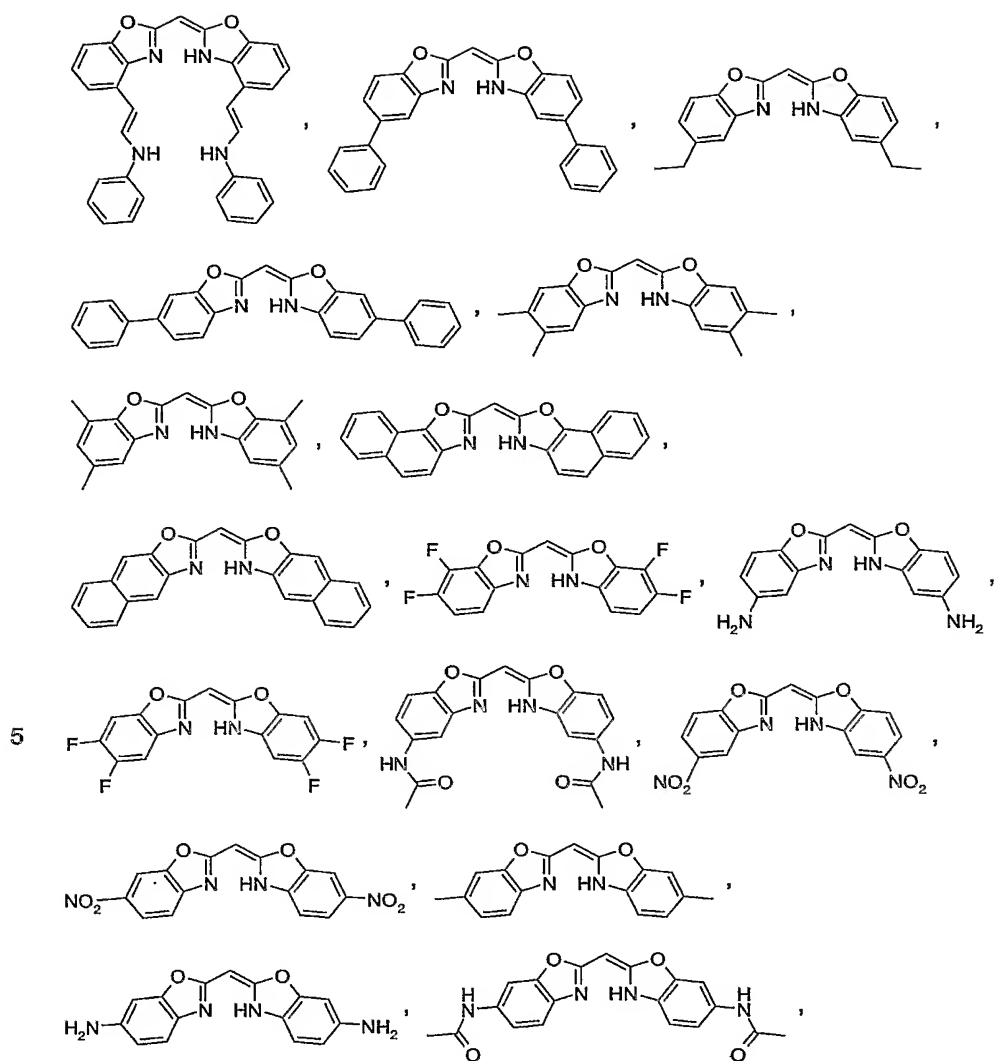


Cu, Co, Ni or Pd and  $Z_1$  is a radical of the following compounds:

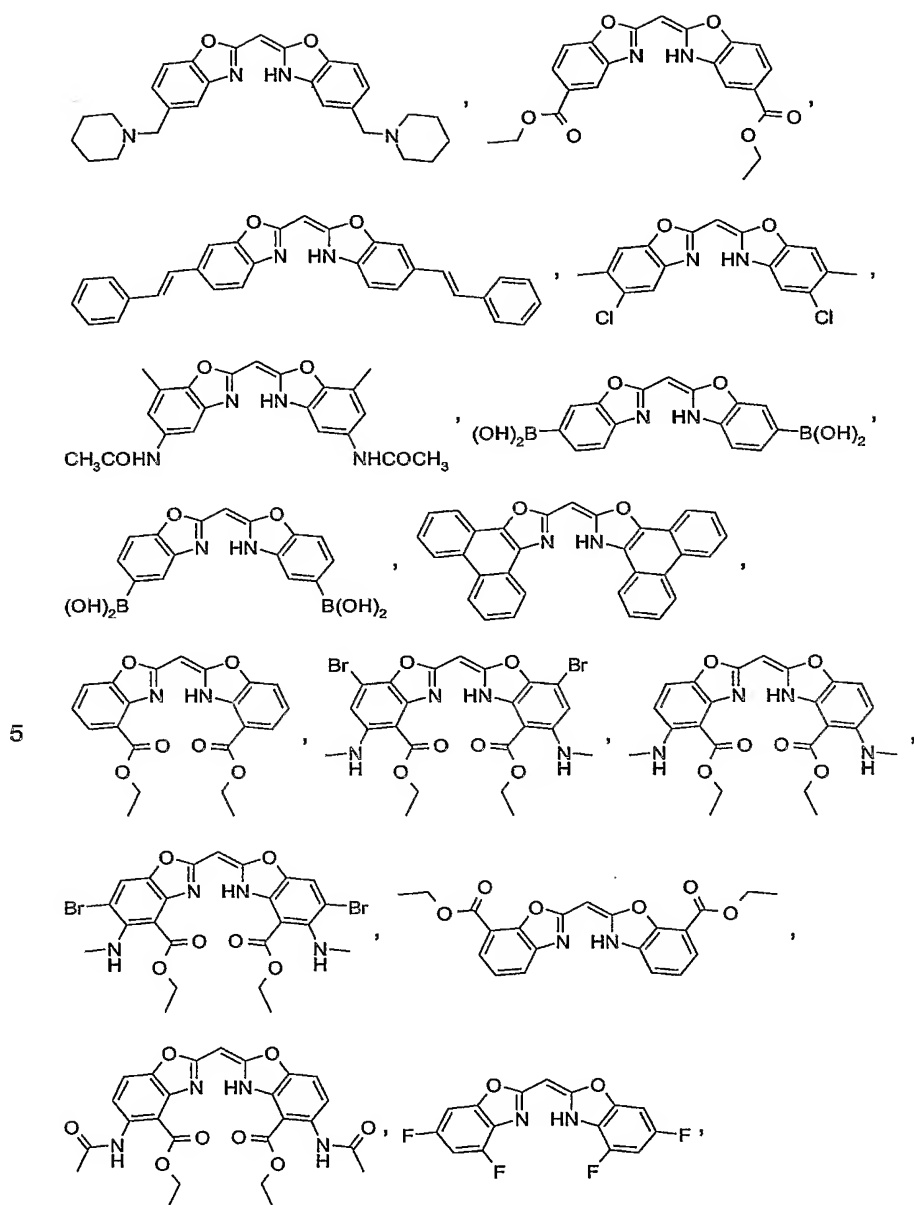


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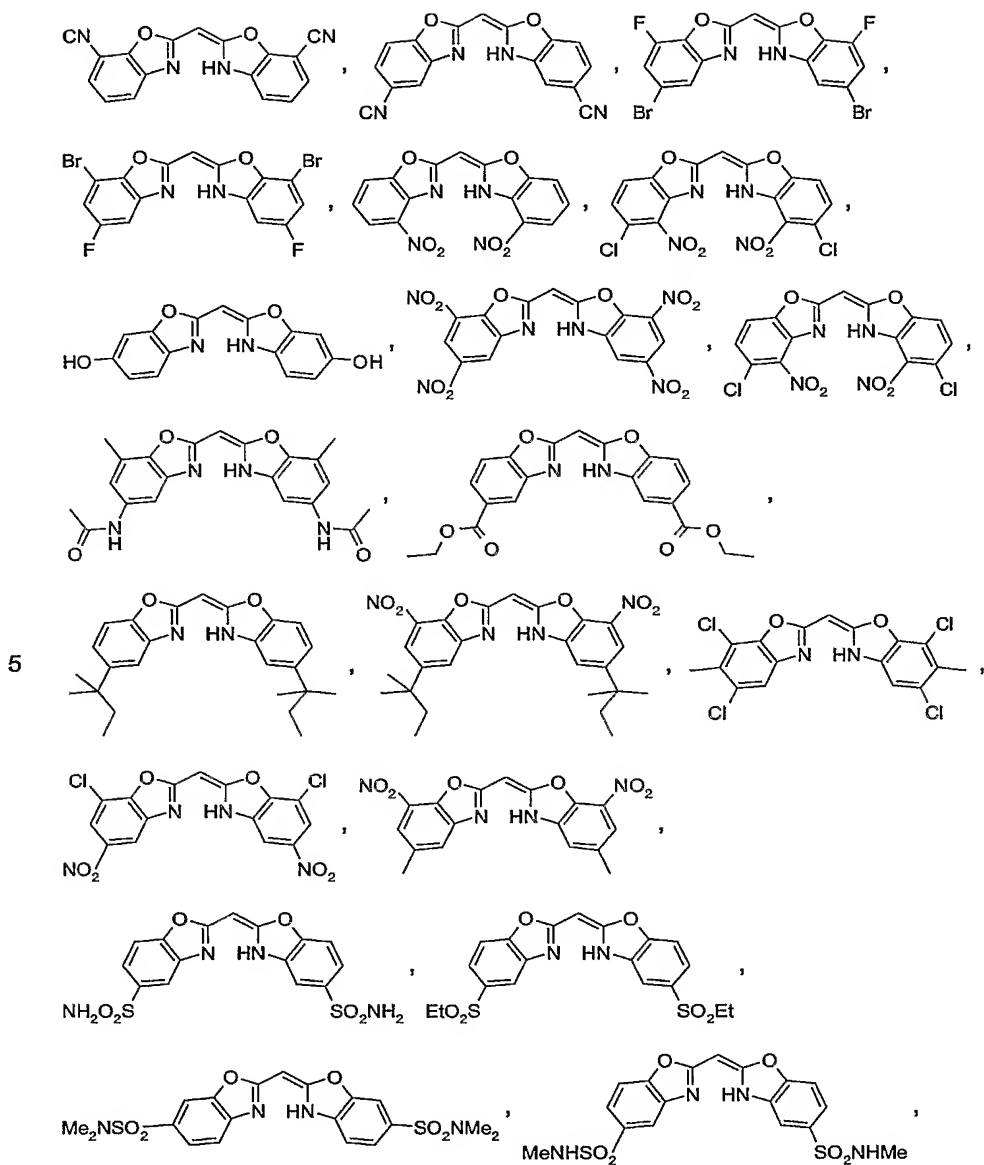




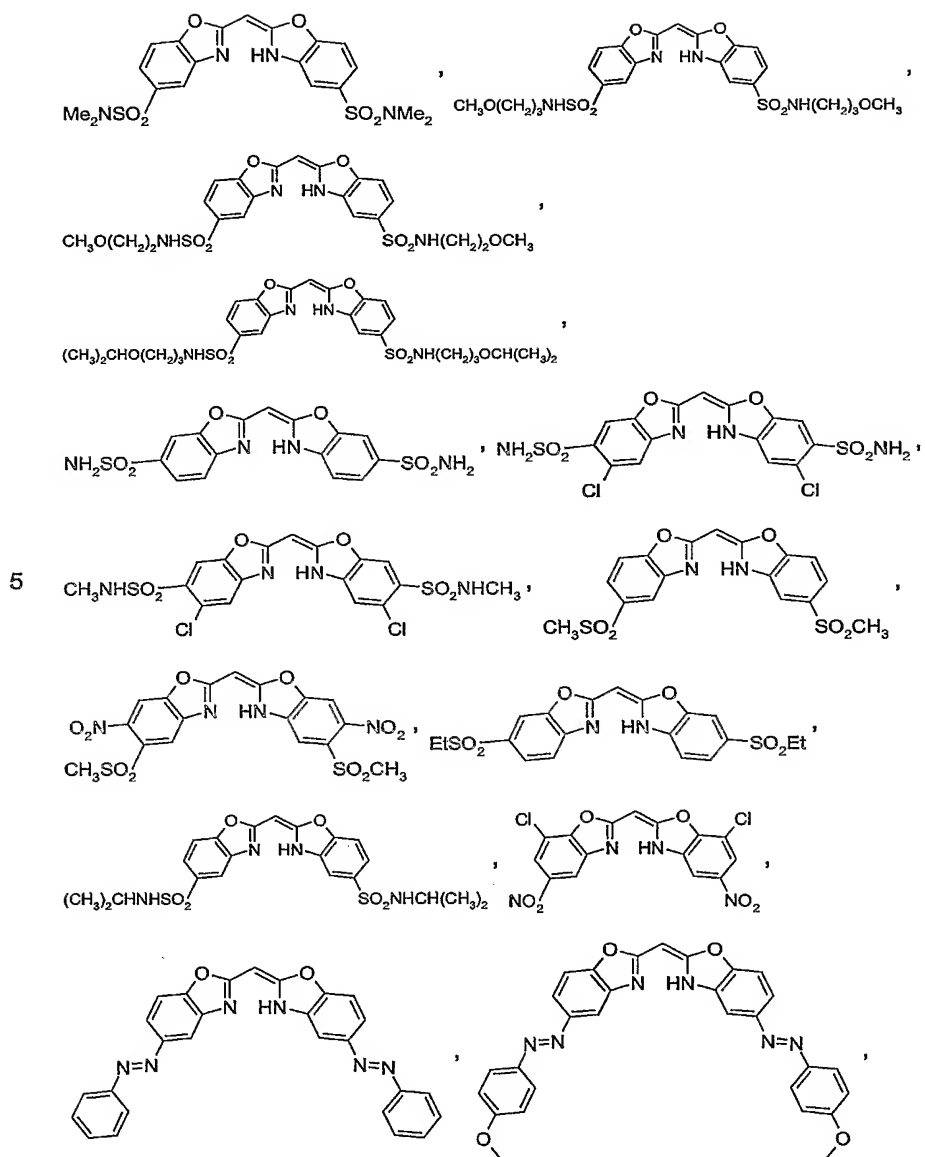
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- 30 -

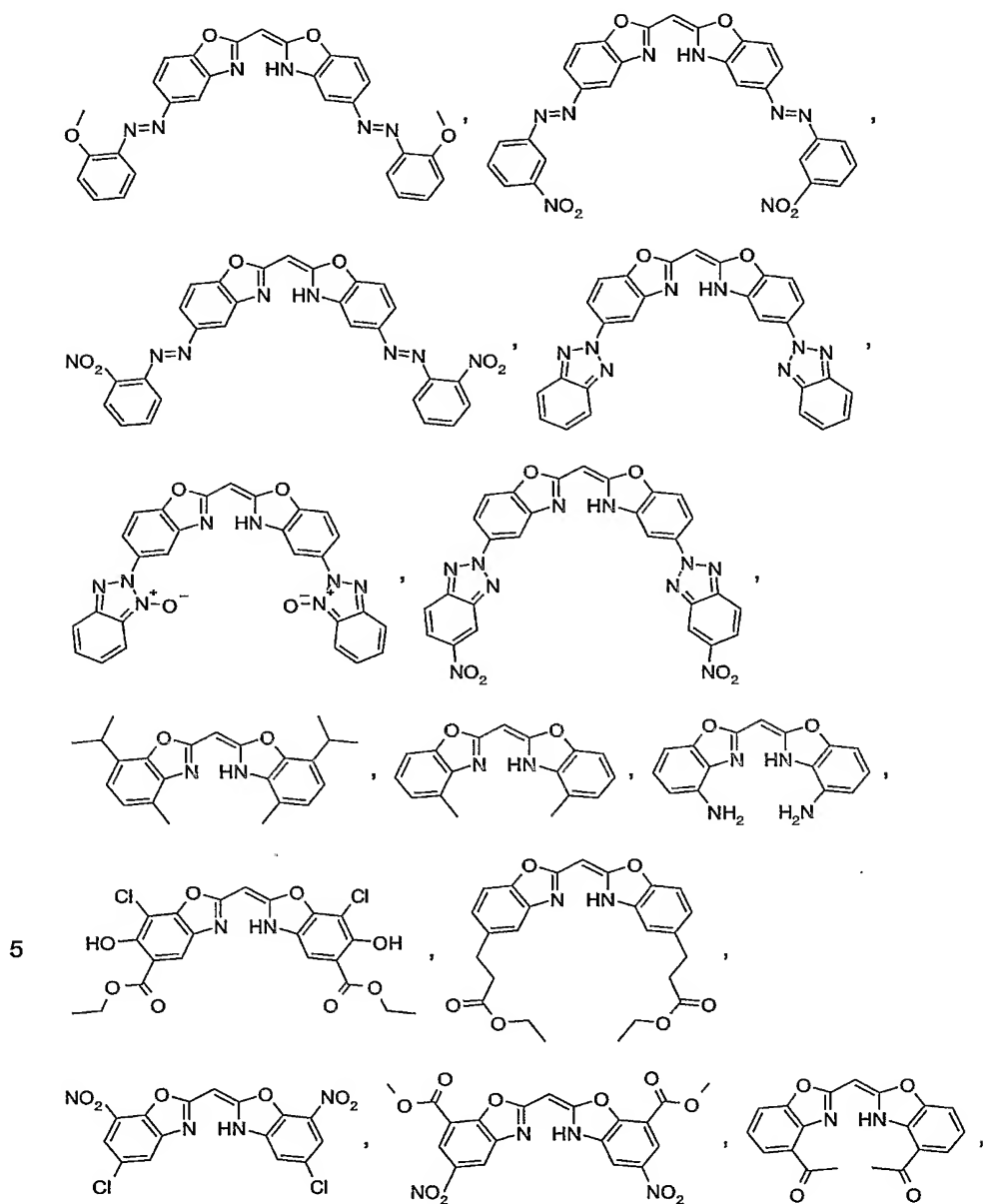


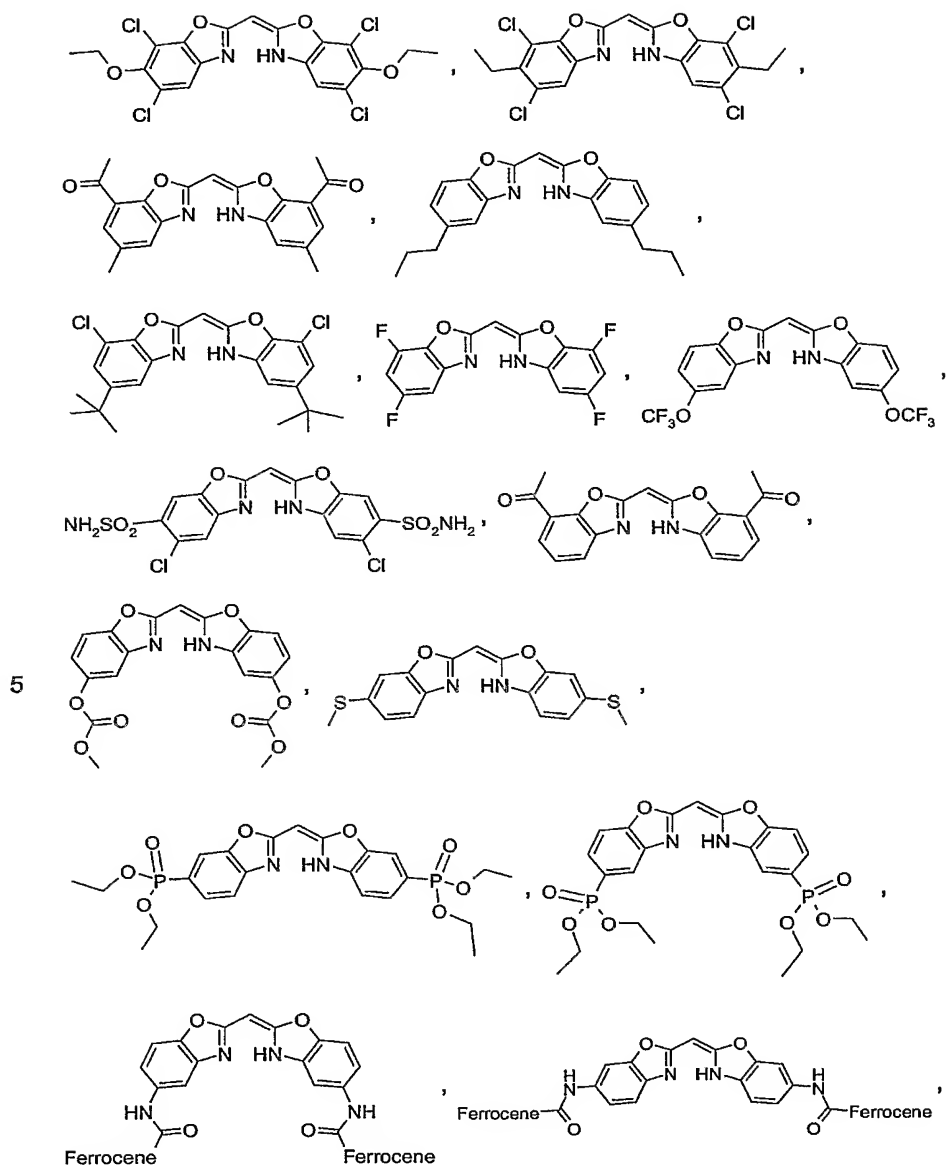
- 31 -



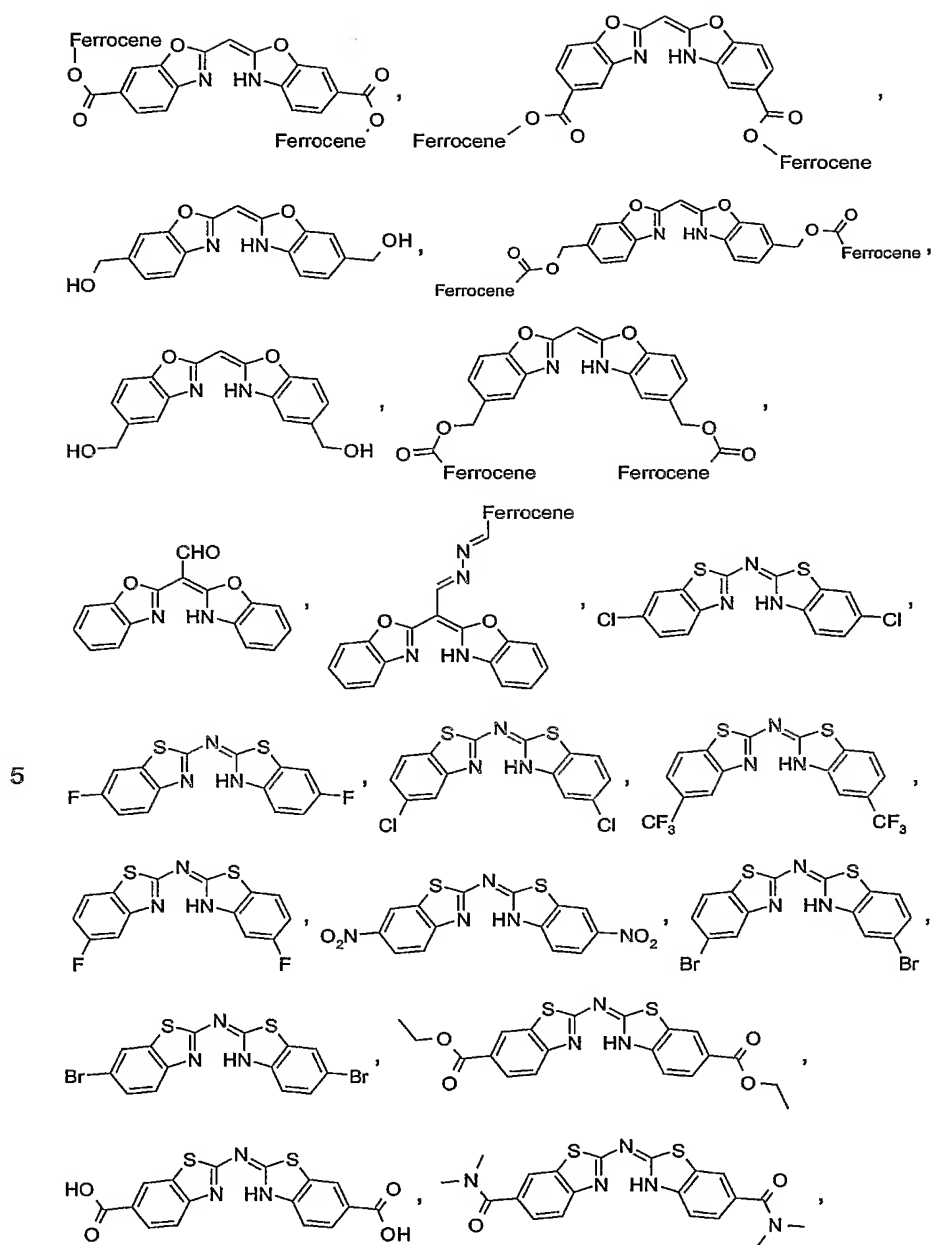


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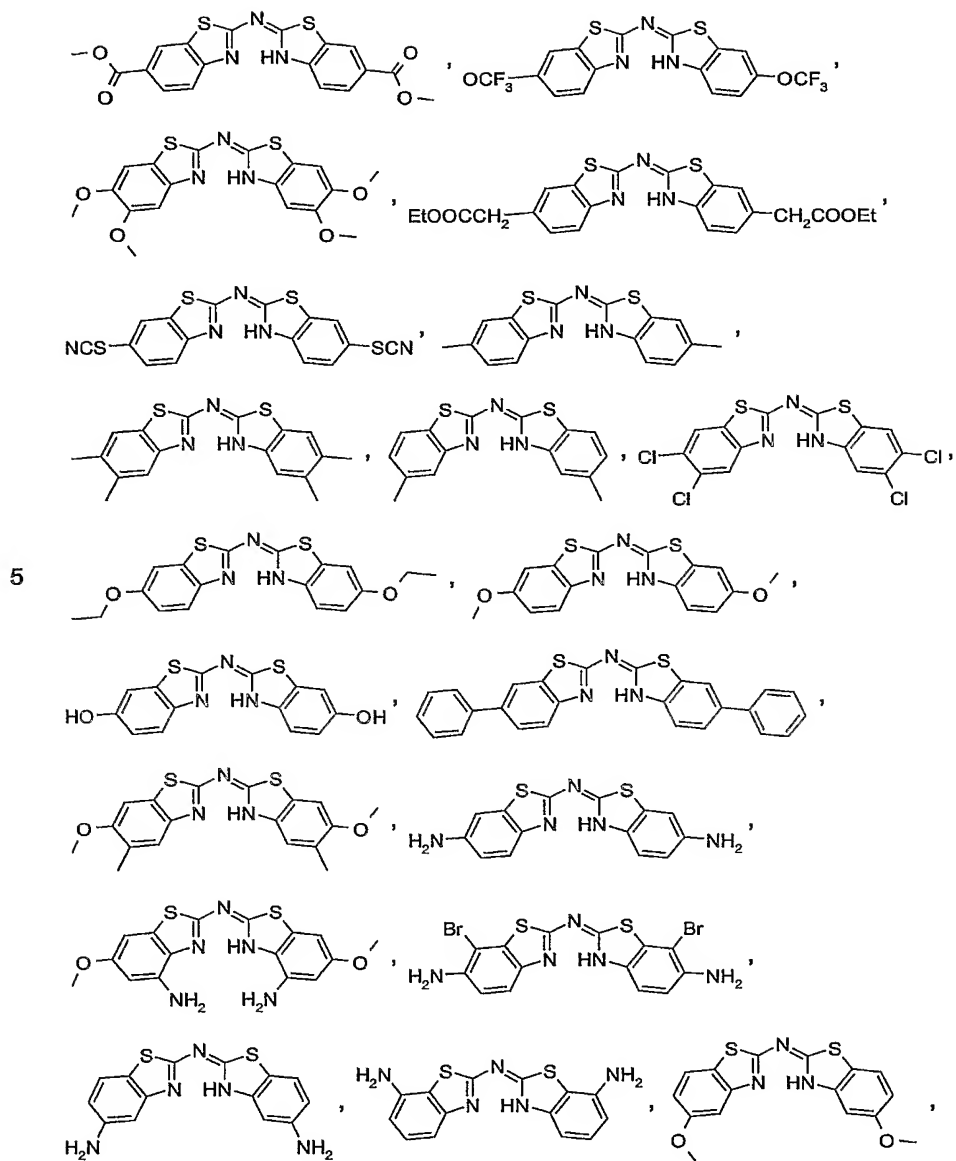




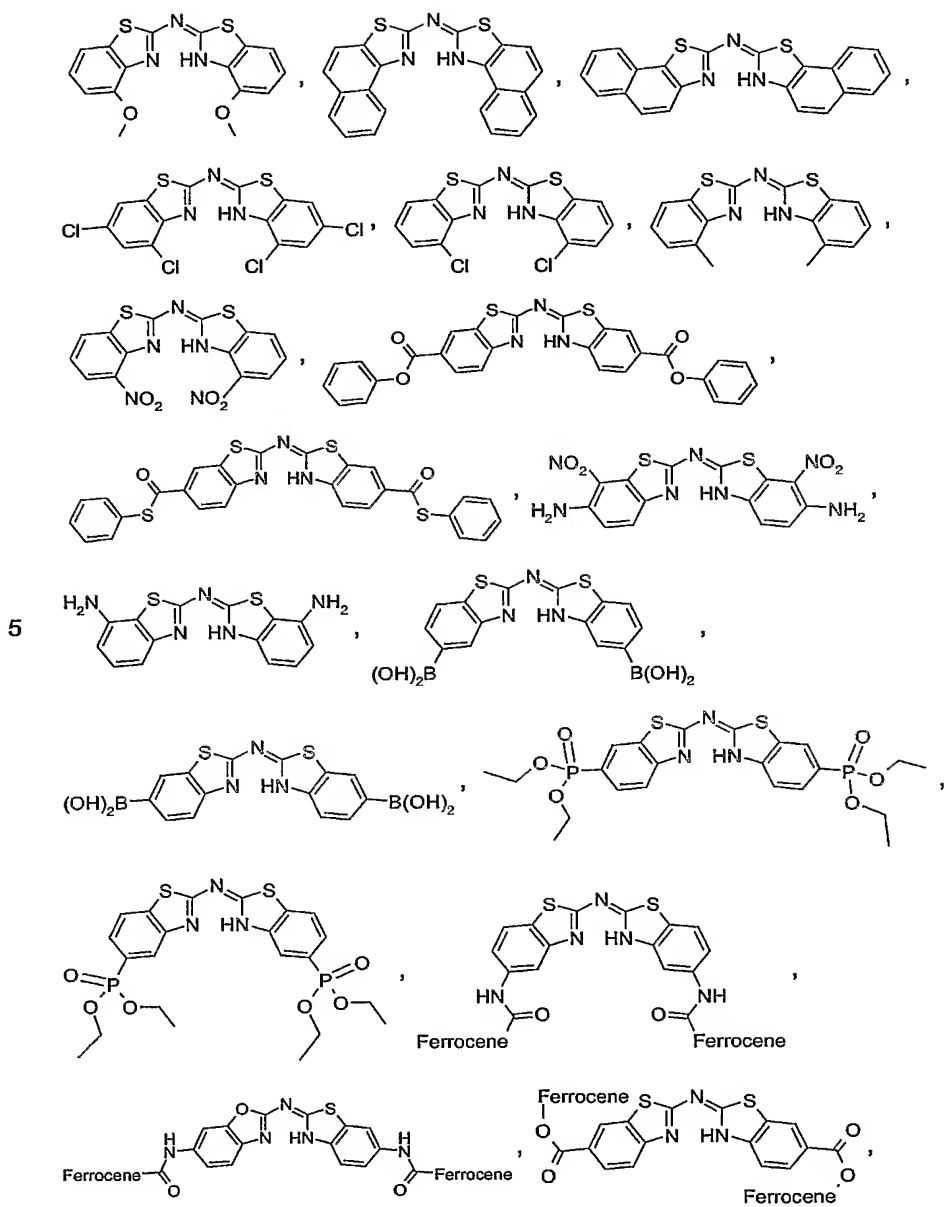
- 34 -



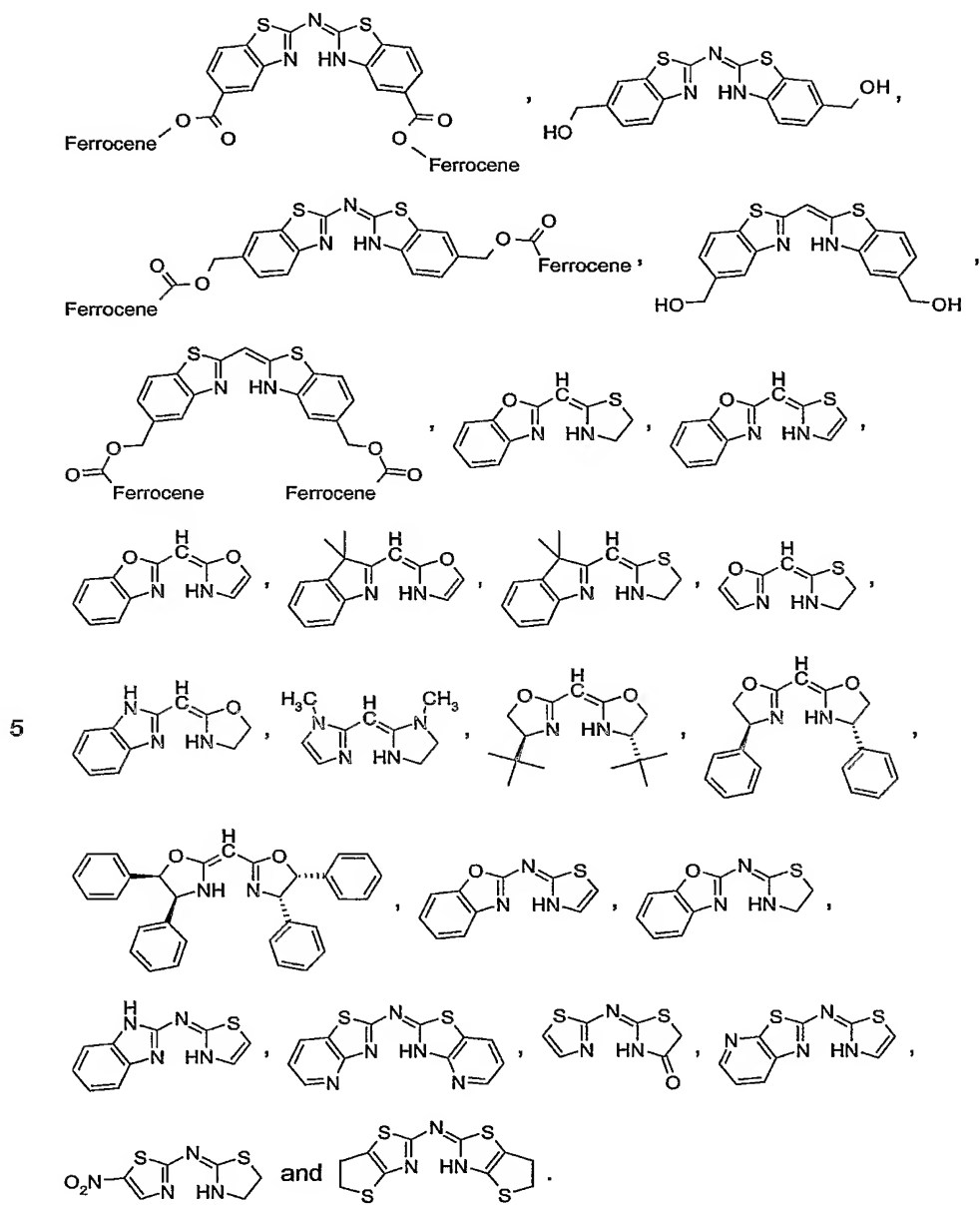
- 35 -



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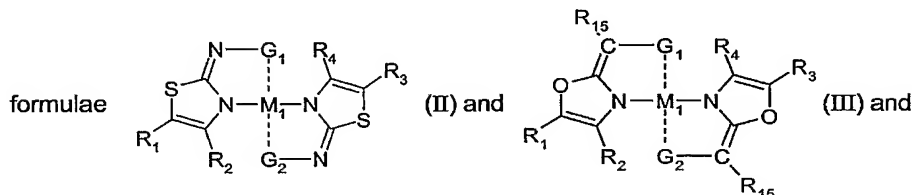


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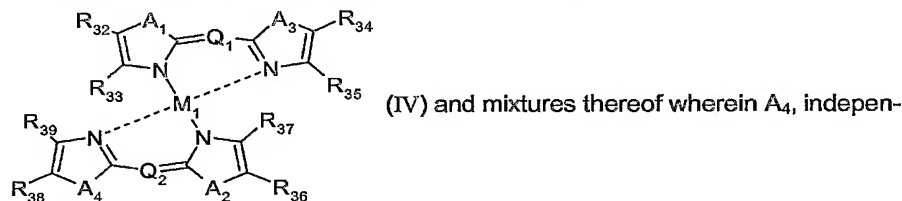
Especially interesting properties are exhibited by the preferred compounds of



also mixtures of compounds of formula (II) and/or (III), wherein especially  $G_1$  and  $G_2$  are the preferred heterocycles disclosed above and at the same time or

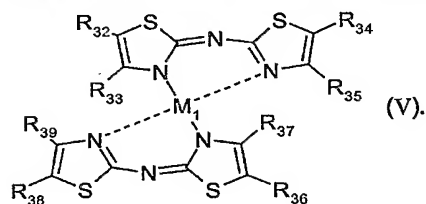
- 5 independently thereof  $M_1$  is a preferred transition metal.  $A_3$  in  $G_1$  and  $G_2$  can be especially N( $R_{12}$ ), O, S or, especially in formula (III), C( $C_1$ - $C_5$ alkyl) $_2$ .

Special preference is given to compounds of formula



dently of  $A_3$ , has the same definition and the same preferred meanings as  $A_3$ .

- 10 Very special preference is given to compounds of formula



Both in formula (IV) and in formula (V),  $R_{32}$ ,  $R_{33}$ ,  $R_{34}$ ,  $R_{35}$ ,  $R_{36}$ ,  $R_{37}$ ,  $R_{38}$  and  $R_{39}$  are preferably H,  $C_1$ - $C_4$ alkyl,  $COO$ - $C_1$ - $C_4$ alkyl, CN,  $NO_2$ , CHO,  $COC_1$ - $C_4$ alkyl, phenyl,  $CH[-O-C_2-C_3$ alkylene-O-],  $C(C_1-C_4$ alkyl) $[-O-C_2-C_3$ alkylene-O-],  $CH=C(CN)_2$ ,

- 15  $C(CN)=C(CN)_2$  or  $C(C_1-C_4$ alkyl) $=C(CN)_2$ , especially H,  $CH_3$ ,  $C_2H_5$ ,  $COOCH_3$ ,

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COOC<sub>2</sub>H<sub>5</sub>, CN, NO<sub>2</sub> or CHO.

Compounds of formula (IV) are, for example, the following:

N°	Formula	A <sub>1</sub> =A <sub>2</sub>	A <sub>3</sub> =A <sub>4</sub>	Q <sub>1</sub> =Q <sub>2</sub>	R <sub>32</sub> =R <sub>36</sub>	R <sub>33</sub> =R <sub>37</sub>	R <sub>34</sub> =R <sub>38</sub>	R <sub>35</sub> =R <sub>39</sub>	M <sub>1</sub>
D1	(IV)	NCH <sub>3</sub>	O	N	H	H	H	H	Co <sup>2+</sup>
D2	(IV)	NCH <sub>2</sub> CH <sub>3</sub>	O	N	CH <sub>3</sub>	H	CH <sub>3</sub>	H	Co <sup>2+</sup>
D3	(IV)	NCH <sub>2</sub> CH <sub>3</sub>	O	N	CH <sub>3</sub>	H	H	H	Co <sup>2+</sup>
D4	(IV)	S	O	N	NO <sub>2</sub>	H	H	H	Co <sup>2+</sup>
D5	(IV)	S	O	N	NO <sub>2</sub>	H	CH <sub>3</sub>	H	Co <sup>2+</sup>
D6	(IV)	NCH <sub>3</sub>	NCH <sub>3</sub>	N	NO <sub>2</sub>	H	NO <sub>2</sub>	H	Co <sup>2+</sup>
D7	(IV)	NCH <sub>2</sub> CH <sub>3</sub>	NCH <sub>2</sub> CH <sub>3</sub>	N	CN	H	CN	H	Co <sup>2+</sup>
D8	(IV)	S	NCH <sub>2</sub> CH <sub>3</sub>	N	H	H	H	H	Co <sup>2+</sup>
D9	(IV)	O	O	CH	NO <sub>2</sub>	H	NO <sub>2</sub>	H	Co <sup>2+</sup>
D10	(IV)	O	O	CH	CN	H	CN	H	Co <sup>2+</sup>
D11	(IV)	O	O	CH	SCH <sub>3</sub>	H	SCH <sub>3</sub>	H	Co <sup>2+</sup>
D12	(IV)	S	S	N	t-C <sub>4</sub> H <sub>9</sub>	H	t-C <sub>4</sub> H <sub>9</sub>	H	Co <sup>2+</sup>
D13	(IV)	S	S	N	CHO	H	CHO	H	Co <sup>2+</sup>
D14	(IV)	S	S	N	H	i-C <sub>3</sub> H <sub>7</sub>	H	i-C <sub>3</sub> H <sub>7</sub>	Co <sup>2+</sup>
D15	(IV)	S	S	N	CHC(CN) <sub>2</sub>	H	CHC(CN) <sub>2</sub>	H	Co <sup>2+</sup>
D16	(IV)	NCH <sub>3</sub>	O	N	H	H	H	H	Cu <sup>2+</sup>
D17	(IV)	NCH <sub>2</sub> CH <sub>3</sub>	O	N	CH <sub>3</sub>	H	CH <sub>3</sub>	H	Cu <sup>2+</sup>
D18	(IV)	NCH <sub>2</sub> CH <sub>3</sub>	O	N	CH <sub>3</sub>	H	H	H	Ni <sup>2+</sup>
D19	(IV)	S	O	N	NO <sub>2</sub>	H	H	H	Cu <sup>2+</sup>
D20	(IV)	S	O	N	NO <sub>2</sub>	H	CH <sub>3</sub>	H	Cu <sup>2+</sup>
D21	(IV)	NCH <sub>3</sub>	NCH <sub>3</sub>	N	NO <sub>2</sub>	H	NO <sub>2</sub>	H	Ni <sup>2+</sup>



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N°	Formula	A <sub>1</sub> =A <sub>2</sub>	A <sub>3</sub> =A <sub>4</sub>	Q <sub>1</sub> =Q <sub>2</sub>	R <sub>32</sub> =R <sub>36</sub>	R <sub>33</sub> =R <sub>37</sub>	R <sub>34</sub> =R <sub>38</sub>	R <sub>35</sub> =R <sub>39</sub>	M <sub>1</sub>
D22	(IV)	NCH <sub>2</sub> CH <sub>3</sub>	NCH <sub>2</sub> CH <sub>3</sub>	N	CN	H	CN	H	Cu <sup>2+</sup>
D23	(IV)	S	NCH <sub>2</sub> CH <sub>3</sub>	N	H	H	H	H	Cu <sup>2+</sup>
D24	(IV)	O	O	CH	NO <sub>2</sub>	H	NO <sub>2</sub>	H	Ni <sup>2+</sup>
D25	(IV)	O	O	CH	CN	H	CN	H	Cu <sup>2+</sup>
D26	(IV)	O	O	CH	SCH <sub>3</sub>	H	SCH <sub>3</sub>	H	Cu <sup>2+</sup>
D27	(IV)	S	S	N	t-C <sub>4</sub> H <sub>9</sub>	H	t-C <sub>4</sub> H <sub>9</sub>	H	Ni <sup>2+</sup>
D28	(IV)	S	S	N	CHO	H	CHO	H	Cu <sup>2+</sup>
D29	(IV)	S	S	N	H	i-C <sub>3</sub> H <sub>7</sub>	H	i-C <sub>3</sub> H <sub>7</sub>	Cu <sup>2+</sup>
D30	(IV)	S	S	N	CHC(CN) <sub>2</sub>	H	CHC(CN) <sub>2</sub>	H	Ni <sup>2+</sup>

Compounds of formula (V) are, for example, the following:

N°	Formula	R <sub>32</sub> =R <sub>36</sub>	R <sub>33</sub> =R <sub>37</sub>	R <sub>34</sub> =R <sub>38</sub>	R <sub>35</sub> =R <sub>39</sub>	M <sub>1</sub>
D31	(V)	H	H	H	H	Co <sup>2+</sup>
D32	(V)	CH <sub>3</sub>	H	CH <sub>3</sub>	H	Co <sup>2+</sup>
D33	(V)	CH <sub>3</sub>	H	H	H	Co <sup>2+</sup>
D34	(V)	H	CH <sub>3</sub>	H	CH <sub>3</sub>	Co <sup>2+</sup>
D35	(V)	H	H	H	CH <sub>3</sub>	Co <sup>2+</sup>
D36	(V)	CH <sub>2</sub> CH <sub>3</sub>	H	CH <sub>2</sub> CH <sub>3</sub>	H	Co <sup>2+</sup>
D37	(V)	CH <sub>2</sub> CH <sub>3</sub>	H	H	H	Co <sup>2+</sup>
D38	(V)	n-C <sub>3</sub> H <sub>7</sub>	H	n-C <sub>3</sub> H <sub>7</sub>	H	Co <sup>2+</sup>
D39	(V)	n-C <sub>3</sub> H <sub>7</sub>	H	H	H	Co <sup>2+</sup>
D40	(V)	i-C <sub>3</sub> H <sub>7</sub>	H	i-C <sub>3</sub> H <sub>7</sub>	H	Co <sup>2+</sup>
D41	(V)	i-C <sub>3</sub> H <sub>7</sub>	H	H	H	Co <sup>2+</sup>

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N°	Formula	R <sub>32</sub> =R <sub>36</sub>	R <sub>33</sub> =R <sub>37</sub>	R <sub>34</sub> =R <sub>38</sub>	R <sub>35</sub> =R <sub>39</sub>	M <sub>1</sub>
D42	(V)	n-C <sub>4</sub> H <sub>9</sub>	H	n-C <sub>4</sub> H <sub>9</sub>	H	Co <sup>2+</sup>
D43	(V)	n-C <sub>4</sub> H <sub>9</sub>	H	H	H	Co <sup>2+</sup>
D44	(V)	i-C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	i-C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	Co <sup>2+</sup>
D45	(V)	H	H	i-C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	Co <sup>2+</sup>
D46	(V)	H	i-C <sub>4</sub> H <sub>9</sub>	H	i-C <sub>4</sub> H <sub>9</sub>	Co <sup>2+</sup>
D47	(V)	H	i-C <sub>4</sub> H <sub>9</sub>	H	H	Co <sup>2+</sup>
D48	(V)	COOCH <sub>2</sub> CH <sub>3</sub>	CH <sub>3</sub>	COOCH <sub>2</sub> CH <sub>3</sub>	CH <sub>3</sub>	Co <sup>2+</sup>
D49	(V)	COOCH <sub>2</sub> CH <sub>3</sub>	CH <sub>3</sub>	H	H	Co <sup>2+</sup>
D50	(V)	H	COOCH <sub>2</sub> CH <sub>3</sub>	H	H	Co <sup>2+</sup>
D51	(V)	H	COOCH <sub>2</sub> CH <sub>3</sub>	H	COOCH <sub>2</sub> CH <sub>3</sub>	Co <sup>2+</sup>
D52	(V)	CH=C(CN) <sub>2</sub>	H	CH=C(CN) <sub>2</sub>	H	Co <sup>2+</sup>
D53	(V)	NO <sub>2</sub>	H	NO <sub>2</sub>	H	Co <sup>2+</sup>
D54	(V)	H	H	H	H	Cu <sup>2+</sup>
D55	(V)	CH <sub>3</sub>	H	CH <sub>3</sub>	H	Cu <sup>2+</sup>
D56	(V)	CH <sub>3</sub>	H	H	H	Cu <sup>2+</sup>
D57	(V)	H	CH <sub>3</sub>	H	CH <sub>3</sub>	Cu <sup>2+</sup>
D58	(V)	H	H	H	CH <sub>3</sub>	Cu <sup>2+</sup>
D59	(V)	CH <sub>2</sub> CH <sub>3</sub>	H	CH <sub>2</sub> CH <sub>3</sub>	H	Cu <sup>2+</sup>
D60	(V)	CH <sub>2</sub> CH <sub>3</sub>	H	H	H	Cu <sup>2+</sup>
D61	(V)	n-C <sub>3</sub> H <sub>7</sub>	H	n-C <sub>3</sub> H <sub>7</sub>	H	Cu <sup>2+</sup>
D62	(V)	n-C <sub>3</sub> H <sub>7</sub>	H	H	H	Cu <sup>2+</sup>
D63	(V)	i-C <sub>3</sub> H <sub>7</sub>	H	i-C <sub>3</sub> H <sub>7</sub>	H	Cu <sup>2+</sup>
D64	(V)	i-C <sub>3</sub> H <sub>7</sub>	H	H	H	Cu <sup>2+</sup>
D65	(V)	n-C <sub>4</sub> H <sub>9</sub>	H	n-C <sub>4</sub> H <sub>9</sub>	H	Cu <sup>2+</sup>

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N°	Formula	R <sub>32</sub> =R <sub>36</sub>	R <sub>33</sub> =R <sub>37</sub>	R <sub>34</sub> =R <sub>38</sub>	R <sub>35</sub> =R <sub>39</sub>	M <sub>1</sub>
D66	(V)	n-C <sub>4</sub> H <sub>9</sub>	H	H	H	Cu <sup>2+</sup>
D67	(V)	i-C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	i-C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	Cu <sup>2+</sup>
D68	(V)	H	H	i-C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	Cu <sup>2+</sup>
D69	(V)	H	i-C <sub>4</sub> H <sub>9</sub>	H	i-C <sub>4</sub> H <sub>9</sub>	Cu <sup>2+</sup>
D70	(V)	H	i-C <sub>4</sub> H <sub>9</sub>	H	H	Cu <sup>2+</sup>
D71	(V)	COOCH <sub>2</sub> CH <sub>3</sub>	CH <sub>3</sub>	COOCH <sub>2</sub> CH <sub>3</sub>	CH <sub>3</sub>	Cu <sup>2+</sup>
D72	(V)	COOCH <sub>2</sub> CH <sub>3</sub>	CH <sub>3</sub>	H	H	Cu <sup>2+</sup>
D73	(V)	H	COOCH <sub>2</sub> CH <sub>3</sub>	H	H	Cu <sup>2+</sup>
D74	(V)	H	COOCH <sub>2</sub> CH <sub>3</sub>	H	COOCH <sub>2</sub> CH <sub>3</sub>	Cu <sup>2+</sup>
D75	(V)	CH=C(CN) <sub>2</sub>	H	CH=C(CN) <sub>2</sub>	H	Cu <sup>2+</sup>
D76	(V)	NO <sub>2</sub>	H	NO <sub>2</sub>	H	Cu <sup>2+</sup>
D77	(V)	H	H	H	H	Ni <sup>2+</sup>
D78	(V)	CH <sub>3</sub>	H	CH <sub>3</sub>	H	Ni <sup>2+</sup>
D79	(V)	CH <sub>3</sub>	H	H	H	Ni <sup>2+</sup>
D80	(V)	H	CH <sub>3</sub>	H	CH <sub>3</sub>	Ni <sup>2+</sup>
D81	(V)	H	H	H	CH <sub>3</sub>	Ni <sup>2+</sup>
D82	(V)	CH <sub>2</sub> CH <sub>3</sub>	H	CH <sub>2</sub> CH <sub>3</sub>	H	Ni <sup>2+</sup>
D83	(V)	CH <sub>2</sub> CH <sub>3</sub>	H	H	H	Ni <sup>2+</sup>
D84	(V)	n-C <sub>3</sub> H <sub>7</sub>	H	n-C <sub>3</sub> H <sub>7</sub>	H	Ni <sup>2+</sup>
D85	(V)	n-C <sub>3</sub> H <sub>7</sub>	H	H	H	Ni <sup>2+</sup>
D86	(V)	i-C <sub>3</sub> H <sub>7</sub>	H	i-C <sub>3</sub> H <sub>7</sub>	H	Ni <sup>2+</sup>
D87	(V)	i-C <sub>3</sub> H <sub>7</sub>	H	H	H	Ni <sup>2+</sup>
D88	(V)	n-C <sub>4</sub> H <sub>9</sub>	H	n-C <sub>4</sub> H <sub>9</sub>	H	Ni <sup>2+</sup>
D89	(V)	n-C <sub>4</sub> H <sub>9</sub>	H	H	H	Ni <sup>2+</sup>

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N°	Formula	R <sub>32</sub> =R <sub>36</sub>	R <sub>33</sub> =R <sub>37</sub>	R <sub>34</sub> =R <sub>38</sub>	R <sub>35</sub> =R <sub>39</sub>	M <sub>1</sub>
D90	(V)	i-C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	i-C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	Ni <sup>2+</sup>
D91	(V)	H	H	i-C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	Ni <sup>2+</sup>
D92	(V)	H	i-C <sub>4</sub> H <sub>9</sub>	H	i-C <sub>4</sub> H <sub>9</sub>	Ni <sup>2+</sup>
D93	(V)	H	i-C <sub>4</sub> H <sub>9</sub>	H	H	Ni <sup>2+</sup>
D94	(V)	COOCH <sub>2</sub> CH <sub>3</sub>	CH <sub>3</sub>	COOCH <sub>2</sub> CH <sub>3</sub>	CH <sub>3</sub>	Ni <sup>2+</sup>
D95	(V)	COOCH <sub>2</sub> CH <sub>3</sub>	CH <sub>3</sub>	H	H	Ni <sup>2+</sup>
D96	(V)	H	COOCH <sub>2</sub> CH <sub>3</sub>	H	H	Ni <sup>2+</sup>
D97	(V)	H	COOCH <sub>2</sub> CH <sub>3</sub>	H	COOCH <sub>2</sub> CH <sub>3</sub>	Ni <sup>2+</sup>
D98	(V)	CH=C(CN) <sub>2</sub>	H	CH=C(CN) <sub>2</sub>	H	Ni <sup>2+</sup>
D99	(V)	NO <sub>2</sub>	H	NO <sub>2</sub>	H	Ni <sup>2+</sup>

Instead of pure compounds it is also possible to use mixtures thereof, for example the following mixtures:

N°		%		%		%		%
M1	D54	80	D77	20				
M2	D32	5	D54	80	D77	15		
M3	D54	80	D55	10	D78	10		
M4	D54	80	D56	15	D79	5		
M5	D54	80	D55	10	D56	10		
M6	D54	80	D56	20				
M7	D54	80	D56	15	D79	5		
M8	D54	90	D57	10				
M9	D54	80	D57	10	D81	10		
M10	D54	80	D58	20				

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N°		%		%		%		%		%
M11	D54	80	D57	10	D58	10				
M12	D54	65	D57	10	D58	5	D77	15	D81	5
M13	D54	90	D59	10						
M14	D54	80	D60	20						
M15	D54	70	D59	5	D60	10	D76	5	D82	5
M16	D56	90	D61	10						
M17	D56	90	D62	10						
M18	D54	90	D68	10						
M19	D54	90	D71	10						
M20	D54	75	D72	15	D76	5	D95	5		
M21	D54	70	D73	20	D76	5	D96	5		
M22	D54	80	D74	20						
M23	D54	80	D55	5	D56	5	D57	5	D76	5
M24	M5	50	M14	30	D58	5	D76	5	D77	10

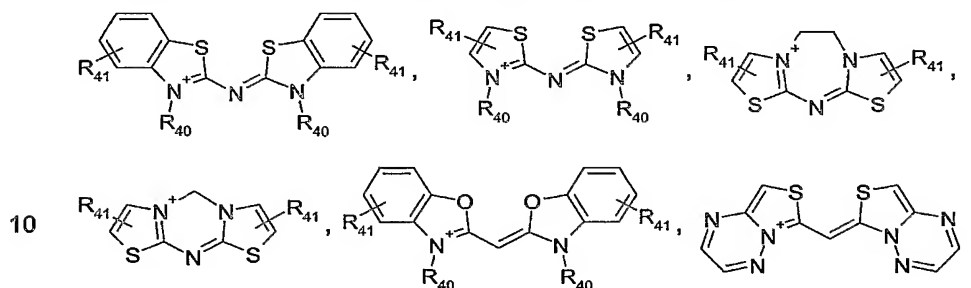
Instead of preparing mixtures by mixing together the components, it is favourably possible to prepare mixtures by mixed synthesis, the metals being added in any desired order in succession or preferably simultaneously to a pre-prepared mixture of the ligands, or conversely the ligands being added in any desired order in succession or preferably all of them simultaneously to a pre-prepared mixture of the metals. The mixtures prepared by mixed synthesis generally have somewhat better solubility than physical mixtures, possibly because of their asymmetric components.

In addition to comprising one or more compounds of formula (I) and optionally customary additives, the optical recording media according to the invention may also comprise other chromophores, preferably metal-free chromophores. Other chromophores may, if desired, be added in an amount of from 1 to 200 % by weight,

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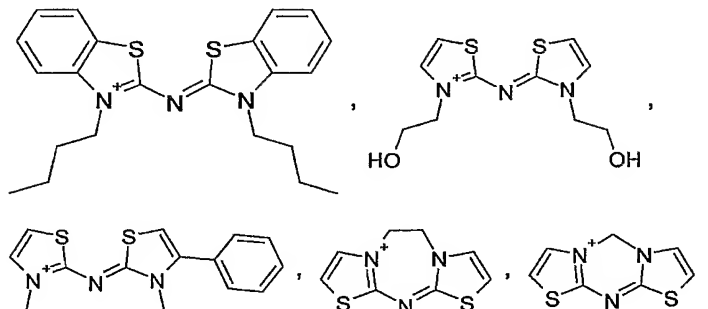
based on the total of the compounds of formula (I). The amount of other chromophores is preferably from 5 to 100 % by weight, especially from 10 to 50 % by weight, based on the total of the compounds of formula (I). Chromophores can be dyes or UV absorbers, preferably having an absorption maximum of from 350 to 400 nm or at from 600 to 700 nm, for example around 380 or 630 nm.

Especially preferred additional metal-free chromophores are cyanines, azacyanines, merocyanines and oxonols and also rhodamines, for example those disclosed in WO 04/006878, WO 02/082438 or EP-A-1 083 555, and also

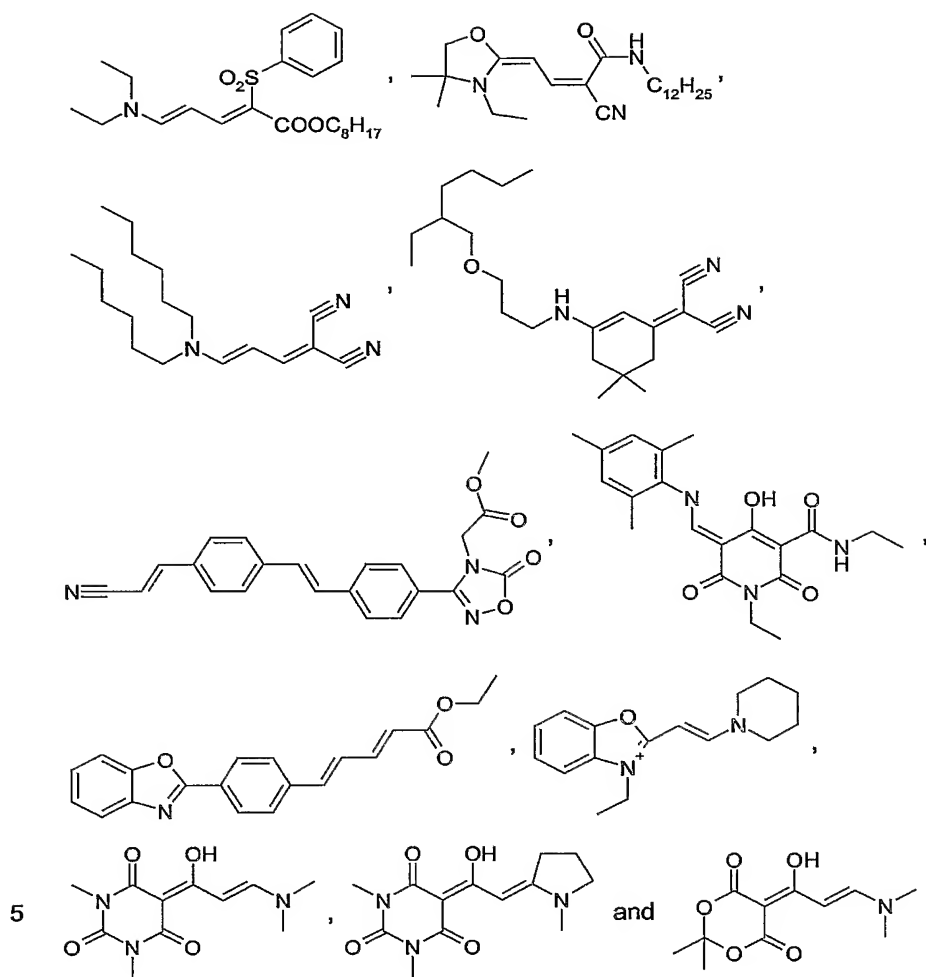


wherein R<sub>40</sub> is C<sub>1</sub>-C<sub>24</sub>alkyl or C<sub>2</sub>-C<sub>24</sub>alkenyl, each of which can be unsubstituted or substituted, and R<sub>41</sub> is any substituent. R<sub>40</sub> may be, for example, methyl, ethyl, vinyl, allyl, isopropyl, n-butyl, 2-isopropoxyethyl, n-pentyl, 3-methyl-butyl, 3,3-dimethyl-butyl, 2-ethyl-hexyl, 2-cyano-ethyl, furan-2-yl-methyl or 2-hydroxy-methyl; R<sub>41</sub> is, for example, C<sub>6</sub>-C<sub>10</sub>aryl, C<sub>1</sub>-C<sub>24</sub>alkyl or C<sub>2</sub>-C<sub>24</sub>alkenyl.

Purely illustrative examples of such chromophores are:



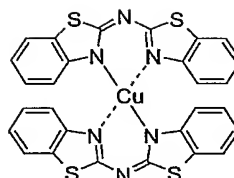
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The following Examples illustrate the invention but do not limit the scope thereof (unless otherwise indicated, “%” always refers to % by weight):

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Example 1: 1.0 g of the compound of formula



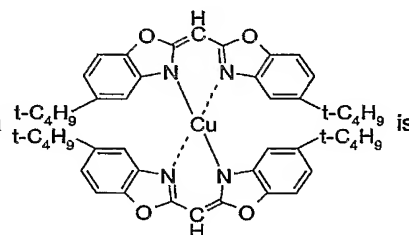
is applied in

the form of a dichloromethane solution to glass. The solid layer is irradiated for 90 hours with xenon light according to ISO-105-B02 (Atlas Ci-35 Weather-O-meter, 15 kJ/cm<sup>2</sup>). The light stability is excellent (see Example 7).

- 5 Example 2: On the solid layer according to Example 1, marks are written into the recording layer using a pulsed dye laser (15 ns pulse length) at a wavelength of 405 nm at an energy density of 0.8 kJ/m<sup>2</sup>. The written sites exhibit a resulting change in reflectivity.

- 10 Example 3: 0.5 g of the compound according to Example 1 is dissolved in 99.5 g of dioxane and applied by means of spin-coating to a silicon wafer. The colourless solid layer is measured using a spectral ellipsometer (Sopra). At a wavelength of 405 nm a refractive index of 2.52 is determined.

Example 4: 1.0 g of the compound of formula



is

dissolved in 99 g of methylcyclohexane and filtered through a 0.2 µm Teflon filter.

- 15 The dye solution is then applied by rotation at 250 rev/min to a 1.2 mm thick, flat polycarbonate plate (diameter 120 mm). The rotational speed is then increased to 1200 rev/min, so that the excess solution is spun off, and a uniform solid layer is formed. After drying, the solid layer has an absorption of 0.61 at 382 nm. Using an optical measuring system (ETA-RT, STEAG ETA-Optik), the layer thickness and the



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complex refractive index are determined. At 405 nm the dye layer has a layer thickness of 56 nm, a refractive index  $n$  of 1.95 and an extinction coefficient  $k$  of 0.090.

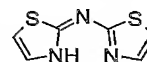
Example 5:

5 Synthesis of the ligand

19.4 ml of a 55 % aqueous chloroacetaldehyde solution are added to a suspension of 10.2 g of dithiobiuret in 45 ml of ethanol. The reaction mixture is heated at 75°C for 2 hours, and then poured into 150 ml of water. After the addition of 200 ml of an aqueous sodium acetate solution (4.6N), the precipitate is filtered off, washed with

10 water and dried at 50°C/ $1.5 \cdot 10^3$  Pa, yielding 8.8 g of crude product, and after

recrystallisation from ethanol 6.7 g of pure product of formula



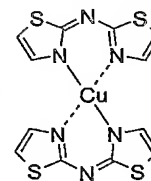
(m.p. 212°C).

Synthesis of the complex

0.5N aqueous copper(II) acetate solution is added to a solution of 458 mg of the

15 resulting ligand in 30 ml of ethanol until precipitation, which begins immediately, is complete. After filtration, the product is washed with ethanol and diethyl ether, and

then dried at 70°C/ $1.5 \cdot 10^3$  Pa. 390 mg of pure product of formula



(decomp. 264°C) are obtained.

Example 6: 1.0 g of the complex according to Example 5 is dissolved in 99 g of

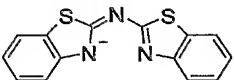
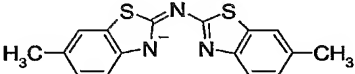
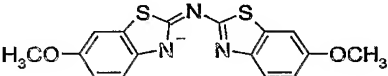
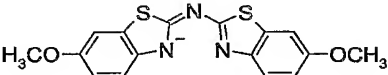
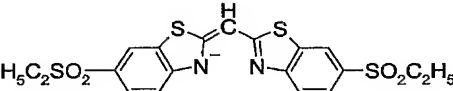
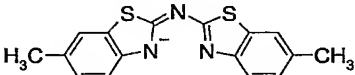
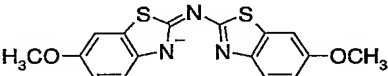
20 2,2,3,3-tetrafluoro-1-propanol and filtered through a 0.2  $\mu$ m Teflon filter. The dye solution is then applied by rotation at 250 rev/min to a 1.2 mm thick, flat polycarbonate plate (diameter 120 mm); the rotational speed is then increased to 1500 rev/min, so that the excess solution is spun off and a uniform solid layer is

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formed. After drying, the solid layer has an absorption of 0.35 at 356 nm. Using an optical measuring system (ETA-RT, STEAG ETA-Optik), the layer thickness and the complex refractive index are determined. At 405 nm the dye layer has a layer thickness of 18 nm, a refractive index  $n$  of 2.25 and an extinction coefficient  $k$  of

5 0.031.

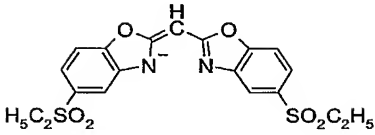
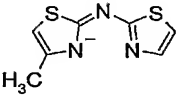
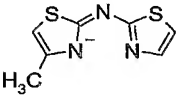
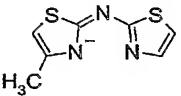
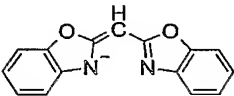
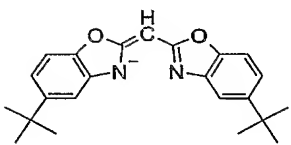
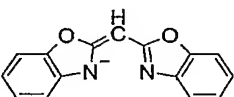
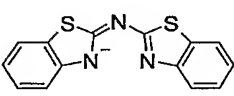
Examples 7 – 38: The procedure is analogous to Example 6, but instead of the complex of Example 5 the following ligands and metal cations are used:

Metal	Ligand (2×)	$\lambda_{\max}$ [nm]	Solvent	$n$	$k$
$\text{Cu}^{2+}$		370	$\text{CH}_3\text{CN}$ (+HCl)	2.52	0.47
$\text{Cu}^{2+}$		383	$\text{CH}_2\text{Cl}_2$	2.30	0.185
$\text{Ni}^{2+}$		370	$\text{CH}_2\text{Cl}_2$	2.23	0.160
$\text{Cu}^{2+}$		390	$\text{CH}_2\text{Cl}_2$	2.22	0.266
$\text{Cu}^{2+}$		377	$\text{CH}_2\text{Cl}_2$	2.21	0.244
$\text{Co}^{2+}$		370	$\text{CH}_2\text{Cl}_2$	2.20	0.137
$\text{Co}^{2+}$		376	$\text{CH}_2\text{Cl}_2$	2.19	0.179

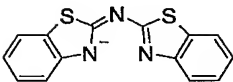
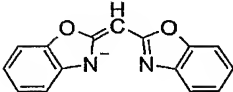
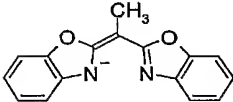
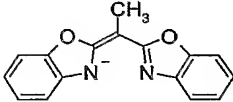
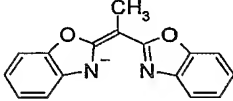
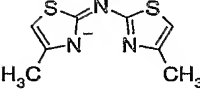
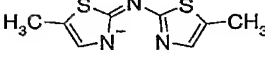
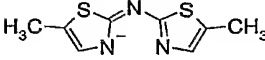
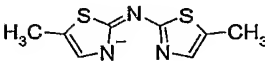
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Metal	Ligand (2×)	$\lambda_{\max}$ [nm]	Solvent	n	k
Ni <sup>2+</sup>		361	CH <sub>2</sub> Cl <sub>2</sub>	2.17	0.108
Co <sup>2+</sup>		370	CH <sub>2</sub> Cl <sub>2</sub>	2.08	0.158
Ni <sup>2+</sup>		361	CH <sub>2</sub> Cl <sub>2</sub>	2.07	0.097
Cu <sup>2+</sup>		384	CH <sub>2</sub> Cl <sub>2</sub>	2.00	0.092
Co <sup>2+</sup>		351	CH <sub>2</sub> Cl <sub>2</sub>	1.98	0.100
Co <sup>2+</sup>		370	CH <sub>2</sub> Cl <sub>2</sub>	1.94	0.083
Ni <sup>2+</sup>		350	CH <sub>2</sub> Cl <sub>2</sub>	1.93	0.083
Co <sup>2+</sup>		367	CH <sub>2</sub> Cl <sub>2</sub>	1.83	0.103

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Metal	Ligand (2x)	$\lambda_{\text{max}}$ [nm]	Solvent	n	k
Ni <sup>2+</sup>		368	CH <sub>2</sub> Cl <sub>2</sub>	1.74	0.119
Cu <sup>2+</sup>		369	CH <sub>2</sub> Cl <sub>2</sub>		
Ni <sup>2+</sup>		350	CH <sub>2</sub> Cl <sub>2</sub>		
Co <sup>2+</sup>		348	CH <sub>2</sub> Cl <sub>2</sub>		
Ni <sup>2+</sup>		356	CH <sub>3</sub> CN		
Ni <sup>2+</sup>		357	CH <sub>2</sub> Cl <sub>2</sub>		
Co <sup>2+</sup>		364	CH <sub>2</sub> Cl <sub>2</sub>		
Co <sup>2+</sup>		370	CH <sub>3</sub> CN (+HCl)		

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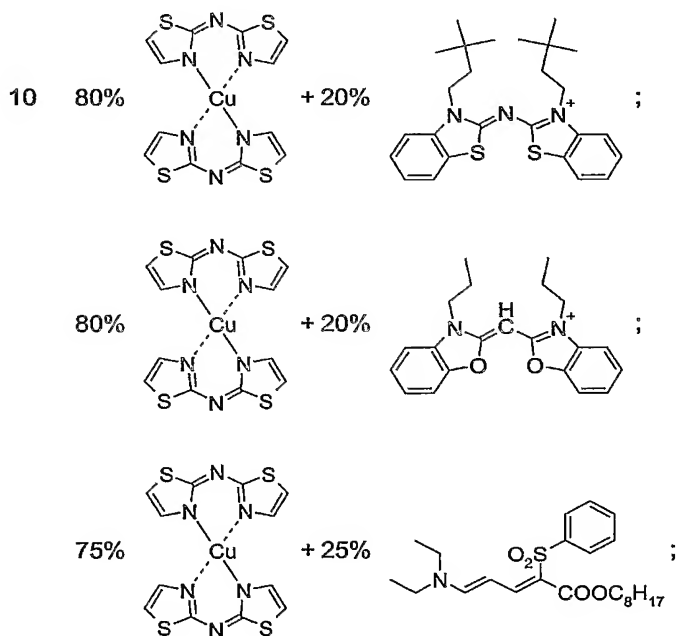
Metal	Ligand (2×)	$\lambda_{\text{max}}$ [nm]	Solvent	n	k
Ni <sup>2+</sup>		370	CH <sub>3</sub> CN (+HCl)		
Cu <sup>2+</sup>		374	CH <sub>2</sub> Cl <sub>2</sub>		
Ni <sup>2+</sup>		374	CH <sub>2</sub> Cl <sub>2</sub>		
Co <sup>2+</sup>		376	CH <sub>3</sub> CN		
Cu <sup>2+</sup>		387	CH <sub>2</sub> Cl <sub>2</sub>		
Cu <sup>2+</sup>					
Ni <sup>2+</sup>					
Co <sup>2+</sup>		350	CH <sub>2</sub> Cl <sub>2</sub>		
Cu <sup>2+</sup>		358	CH <sub>2</sub> Cl <sub>2</sub>		

Examples 39 – 62: The procedure is analogous to Example 6, but instead of the complex of Example 5 the mixtures M1 to M24 are used.

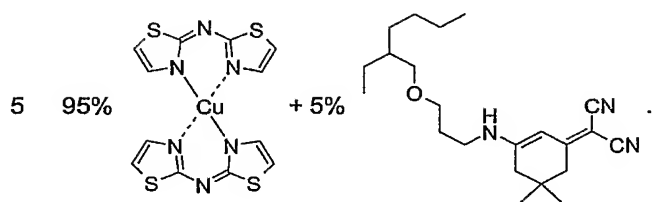
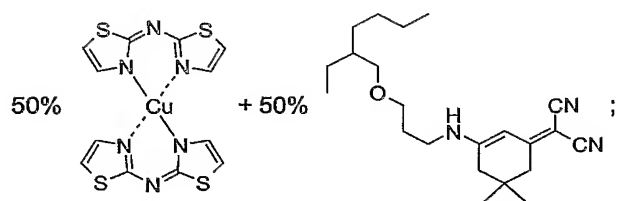
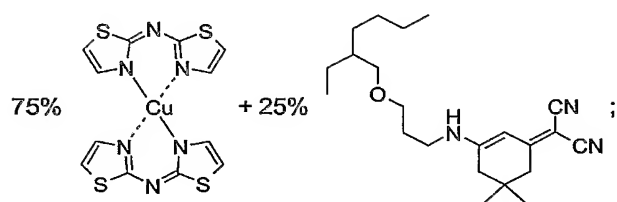
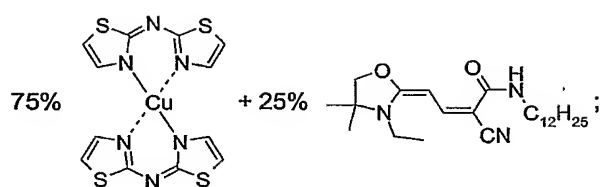
- 53 -

Examples 63 – 86: The procedure is analogous to Example 6, but instead of the complex of Example 5 there are used mixtures having the same proportions of metal and ligand as mixtures M1 to M24 but the complexes are prepared by mixed synthesis (variant of the simultaneous addition of the metal mixture to the ligand mixture). The results are similar to those of Examples 39 – 62, but have surprisingly better solubility and solution stability.

Examples 87 – 94: The procedure is analogous to Example 6, but instead of the complex of Example 5 there are used the following mixtures of compounds of formula (I) with cyanines and merocyanines:



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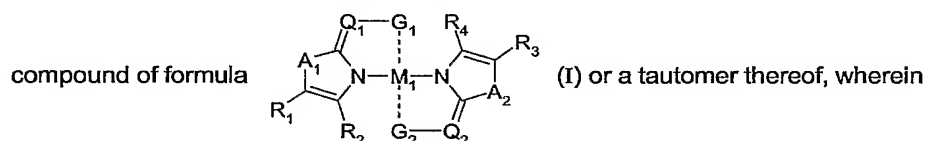
It will be understood that it is also possible to combine mixtures of those cyanines, merocyanines and/or also other chromophores with complexes of formula (I) or with mixtures of complexes of formula (I), the results achieved generally being very good.



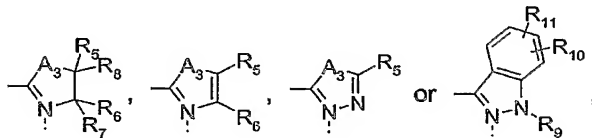
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What is claimed is:

1. An optical recording medium comprising a substrate, a recording layer and optionally one or more reflecting layers, wherein the recording layer comprises a



5  $G_1$  and  $G_2$  are each independently of the other



$A_1$  and  $A_2$  are each independently of the other  $N(R_{12})$ , O, S or Se and  $A_3$  is  $C(C_1-C_5\text{alkyl})_2$ ,  $C(C_4-C_5\text{alkylene})$ ,  $N(R_{12})$ , O, S, Se,  $N=C(R_{13})$  or unsubstituted or  $R_{14}$ -substituted  $CH=CH$ ;

10  $M_1$  is a transition metal of groups IX to XII, preferably Co, Cu, Ni, Pd or Zn, especially Co, Cu or Ni;

$Q_1$  and  $Q_2$  are each independently of the other  $C(R_{15})$ , N or P;

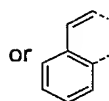
$R_1$ ,  $R_2$ ,  $R_3$ ,  $R_4$ ,  $R_5$ ,  $R_6$ ,  $R_7$ ,  $R_8$  and  $R_{14}$  are each independently of the others hydrogen,  $R_{18}$ , or  $C_6-C_{12}\text{aryl}$ ,  $C_4-C_{12}\text{heteroaryl}$ ,  $C_7-C_{12}\text{aralkyl}$  or  $C_5-C_{12}\text{heteroaralkyl}$

15 each unsubstituted or substituted by one or more, where applicable identical or different, radicals  $R_{18}$ ; or

$R_1$  and  $R_2$ ,  $R_3$  and  $R_4$ ,  $R_5$  and  $R_6$ ,  $R_5$  and  $R_{13}$  and/or  $R_5$  and  $R_{14}$ , together in pairs, are  $C_3-C_6\text{alkylene}$  or  $C_3-C_6\text{alkenylene}$ , each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals  $R_{17}$  and may be

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uninterrupted or interrupted by O, S or N(R<sub>12</sub>), or 1,4-buta-1,3-dienylene,



or , each of which is unsubstituted or substituted by one or more, where

applicable identical or different, radicals R<sub>18</sub> and in which 1 or 2 carbon atoms may have been replaced by nitrogen;

- 5 R<sub>9</sub>, R<sub>12</sub> and R<sub>13</sub> are each independently of the others C<sub>1</sub>-C<sub>24</sub>alkyl, C<sub>3</sub>-C<sub>24</sub>cycloalkyl, C<sub>2</sub>-C<sub>24</sub>alkenyl, C<sub>3</sub>-C<sub>24</sub>cycloalkenyl, C<sub>1</sub>-C<sub>4</sub>alkyl-[O-C<sub>1</sub>-C<sub>4</sub>alkylene]<sub>m</sub> or C<sub>1</sub>-C<sub>4</sub>alkyl-[NH-C<sub>1</sub>-C<sub>4</sub>alkylene]<sub>m</sub>, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R<sub>17</sub>; or C<sub>6</sub>-C<sub>12</sub>aryl, C<sub>4</sub>-C<sub>12</sub>heteroaryl, C<sub>7</sub>-C<sub>12</sub>aralkyl or C<sub>5</sub>-C<sub>12</sub>heteroaralkyl, each of which is unsubstituted or substituted by
- 10 one or more, where applicable identical or different, radicals R<sub>18</sub>;

R<sub>10</sub>, R<sub>11</sub> and R<sub>18</sub> are each independently of the others halogen, nitro, cyano, thiocyanato, hydroxy, O-R<sub>19</sub>, O-CO-R<sub>19</sub>, S-R<sub>19</sub>, CHO, COR<sub>20</sub>, CHOR<sub>19</sub>OR<sub>23</sub>, CR<sub>20</sub>OR<sub>19</sub>OR<sub>23</sub>, R<sub>16</sub>, N=N-R<sub>16</sub>, N=CR<sub>19</sub>R<sub>20</sub>, N=CR<sub>21</sub>R<sub>22</sub>, C(R<sub>15</sub>)=NR<sub>19</sub>, C(R<sub>15</sub>)=NR<sub>21</sub>, C(R<sub>15</sub>)=CR<sub>21</sub>R<sub>22</sub>, NH<sub>2</sub>, NH-R<sub>19</sub>, NR<sub>19</sub>R<sub>20</sub>, NH<sub>3</sub><sup>+</sup>, NH<sub>2</sub>R<sub>19</sub><sup>+</sup>, NHR<sub>19</sub>R<sub>20</sub><sup>+</sup>, NR<sub>19</sub>R<sub>20</sub>R<sub>23</sub><sup>+</sup>, CONH<sub>2</sub>, CONHR<sub>19</sub>, CONR<sub>19</sub>R<sub>20</sub>, SO<sub>2</sub>R<sub>19</sub>, SO<sub>2</sub>NH<sub>2</sub>, SO<sub>2</sub>NHR<sub>19</sub>, SO<sub>2</sub>NR<sub>19</sub>R<sub>20</sub>, COOH, COOR<sub>19</sub>, OCOOR<sub>19</sub>, NHCOR<sub>19</sub>, NR<sub>19</sub>COR<sub>23</sub>, NHCOOR<sub>19</sub>, NR<sub>19</sub>COOR<sub>23</sub>, ureido, NR<sub>19</sub>-CO-NHR<sub>23</sub>, B(OH)<sub>2</sub>, B(OH)(OR<sub>19</sub>), B(OR<sub>19</sub>)OR<sub>23</sub>, phosphato, PR<sub>19</sub>R<sub>23</sub>, POR<sub>19</sub>OR<sub>23</sub>, P(=O)OR<sub>19</sub>OR<sub>23</sub>, OPR<sub>19</sub>R<sub>23</sub>, OPR<sub>19</sub>OR<sub>23</sub>, OP(=O)R<sub>19</sub>OR<sub>23</sub>, OP(=O)OR<sub>19</sub>OR<sub>23</sub>, OPO<sub>3</sub>R<sub>19</sub>, sulfato, sulfo, or C<sub>1</sub>-C<sub>12</sub>alkyl,

- 15 C<sub>3</sub>-C<sub>12</sub>cycloalkyl, C<sub>1</sub>-C<sub>12</sub>alkylthio, C<sub>3</sub>-C<sub>12</sub>cycloalkylthio, C<sub>1</sub>-C<sub>12</sub>alkoxy or C<sub>3</sub>-C<sub>12</sub>cycloalkoxy each unsubstituted or substituted by one or more, where applicable identical or different, radicals R<sub>17</sub>;

R<sub>15</sub> is hydrogen, cyano, hydroxy, C<sub>1</sub>-C<sub>12</sub>alkoxy, C<sub>3</sub>-C<sub>12</sub>cycloalkoxy, C<sub>1</sub>-C<sub>12</sub>alkylthio, C<sub>3</sub>-C<sub>12</sub>cycloalkylthio, amino, NHR<sub>24</sub>, NR<sub>25</sub>R<sub>26</sub>, R<sub>27</sub>, halogen, nitro, formyl, N=N-R<sub>27</sub>,

- 25 C(R<sub>14</sub>)=CR<sub>21</sub>R<sub>22</sub>, C(R<sub>14</sub>)=NR<sub>19</sub>, COO-R<sub>25</sub>, carboxy, carbamoyl, CONH-R<sub>25</sub>,

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CONR<sub>25</sub>R<sub>26</sub>, N=CR<sub>19</sub>R<sub>20</sub>, or C<sub>1</sub>-C<sub>12</sub>alkyl, C<sub>3</sub>-C<sub>12</sub>cycloalkyl, C<sub>2</sub>-C<sub>12</sub>alkenyl or C<sub>3</sub>-C<sub>12</sub>cycloalkenyl each unsubstituted or substituted by one or more, where applicable identical or different, halogen, hydroxy, C<sub>1</sub>-C<sub>12</sub>alkoxy or C<sub>3</sub>-C<sub>12</sub>cycloalkoxy radicals;

- 5 R<sub>16</sub> is C<sub>6</sub>-C<sub>12</sub>aryl, C<sub>4</sub>-C<sub>12</sub>heteroaryl, C<sub>7</sub>-C<sub>12</sub>aralkyl or C<sub>5</sub>-C<sub>12</sub>heteroaralkyl, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals R<sub>28</sub>;

- R<sub>17</sub> is halogen, hydroxy, O-R<sub>25</sub>, O-CO-R<sub>25</sub>, S-R<sub>25</sub>, NH<sub>2</sub>, NH-R<sub>25</sub>, NR<sub>25</sub>R<sub>26</sub>, NH<sub>3</sub><sup>+</sup>, NH<sub>2</sub>R<sub>25</sub><sup>+</sup>, NHR<sub>25</sub>R<sub>26</sub><sup>+</sup>, NR<sub>24</sub>R<sub>25</sub>R<sub>26</sub><sup>+</sup>, NR<sub>25</sub>-CO-R<sub>24</sub>, NR<sub>25</sub>COOR<sub>24</sub>, cyano, formyl,  
 10 COO-R<sub>25</sub>, carboxy, carbamoyl, CONH-R<sub>25</sub>, CONR<sub>25</sub>R<sub>26</sub>, ureido, NH-CO-NHR<sub>24</sub>, NR<sub>25</sub>-CO-NHR<sub>24</sub>, phosphato, PR<sub>25</sub>R<sub>24</sub>, POR<sub>25</sub>OR<sub>24</sub>, P(=O)OR<sub>25</sub>OR<sub>24</sub>, OPR<sub>25</sub>R<sub>24</sub>, OPR<sub>25</sub>OR<sub>24</sub>, OP(=O)R<sub>25</sub>OR<sub>24</sub>, OPO<sub>3</sub>R<sub>25</sub>, OP(=O)OR<sub>25</sub>OR<sub>24</sub>, SO<sub>2</sub>R<sub>25</sub>, sulfato, sulfo, R<sub>27</sub>, N=N-R<sub>27</sub>, or C<sub>1</sub>-C<sub>12</sub>alkoxy or C<sub>1</sub>-C<sub>12</sub>cycloalkoxy each unsubstituted or mono- or poly-substituted by halogen;

- 15 R<sub>19</sub>, R<sub>20</sub> and R<sub>23</sub> are each independently of the others R<sub>16</sub>, or C<sub>1</sub>-C<sub>12</sub>alkyl, C<sub>3</sub>-C<sub>12</sub>cycloalkyl, C<sub>2</sub>-C<sub>12</sub>alkenyl or C<sub>3</sub>-C<sub>12</sub>cycloalkenyl, each of which is unsubstituted or substituted by one or more, where applicable identical or different, halogen, hydroxy, C<sub>1</sub>-C<sub>12</sub>alkoxy or C<sub>3</sub>-C<sub>12</sub>cycloalkoxy radicals; or

- R<sub>14</sub> and R<sub>19</sub> together, R<sub>15</sub> and R<sub>19</sub> together and/or R<sub>19</sub> and R<sub>23</sub> together are  
 20 C<sub>2</sub>-C<sub>12</sub>alkylene, C<sub>3</sub>-C<sub>12</sub>cycloalkylene, C<sub>2</sub>-C<sub>12</sub>alkenylene or C<sub>3</sub>-C<sub>12</sub>cycloalkenylene, each of which is unsubstituted or substituted by one or more, where applicable identical or different, halogen, hydroxy, C<sub>1</sub>-C<sub>12</sub>alkoxy or C<sub>3</sub>-C<sub>12</sub>cycloalkoxy radicals;  
 or

- R<sub>19</sub> and R<sub>20</sub> together with the common nitrogen are pyrrolidine, piperidine, piperazine  
 25 or morpholine, each of which is unsubstituted or mono- to tetra-substituted by C<sub>1</sub>-C<sub>4</sub>alkyl; or carbazole, phenoxazine or phenothiazine, each of which is unsubstituted or substituted by one or more, where applicable identical or different,

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radicals  $R_{28}$ ;

$R_{21}$  and  $R_{22}$  are each independently of the other  $NR_{25}R_{26}$ , CN,  $CONH_2$ ,  $CONHR_{19}$ ,  $CONR_{19}R_{20}$  or  $COOR_{20}$ ;

- $R_{24}$ ,  $R_{25}$  and  $R_{26}$  are each independently of the others  $C_1$ - $C_{12}$ alkyl,  $C_3$ - $C_{12}$ cycloalkyl,   
 5  $C_2$ - $C_{12}$ alkenyl,  $C_3$ - $C_{12}$ cycloalkenyl,  $C_6$ - $C_{12}$ aryl,  $C_4$ - $C_{12}$ heteroaryl,  $C_7$ - $C_{12}$ aralkyl or  $C_5$ - $C_{12}$ heteroaralkyl; or

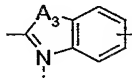
$R_{25}$  and  $R_{26}$  together with the common nitrogen are pyrrolidine, piperidine, piperazine or morpholine, each of which is unsubstituted or mono- to tetra-substituted by  $C_1$ - $C_4$ alkyl;

- 10  $R_{27}$  is  $C_6$ - $C_{12}$ aryl,  $C_4$ - $C_{12}$ heteroaryl,  $C_7$ - $C_{12}$ aralkyl or  $C_5$ - $C_{12}$ heteroaralkyl, each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals  $R_{18}$ ;

- $R_{28}$  is nitro,  $SO_2NHR_{25}$ ,  $SO_2NR_{25}R_{26}$ , or  $C_1$ - $C_{12}$ alkyl,  $C_3$ - $C_{12}$ cycloalkyl,  $C_1$ - $C_{12}$ alkylthio,  $C_3$ - $C_{12}$ cycloalkylthio,  $C_1$ - $C_{12}$ alkoxy or  $C_3$ - $C_{12}$ cycloalkoxy, each of which is   
 15 unsubstituted or substituted by one or more, where applicable identical or different, radicals  $R_{17}$ ; and

$m$  is a number from 1 to 10.

2. An optical recording medium according to claim 1, wherein  $Q_1$  and  $Q_2$  are  $C(R_{15})$ ;

$G_1$  and  $G_2$  are ; and  $A_1$ ,  $A_2$  and  $A_3$  are O, S or  $N(R_{12})$ ;

- 20  $R_{12}$  is  $C_1$ - $C_{24}$ alkyl,  $C_1$ - $C_4$ alkyl- $[O-C_1-C_4$ alkylene] $_m$  or  $C_1$ - $C_4$ alkyl- $[NH-C_1-C_4$ alkylene] $_m$ , each of which is unsubstituted or substituted by one or more, where applicable identical or different, radicals  $R_{17}$ , or  $C_6$ - $C_{12}$ aryl unsubstituted or substituted by one or more, where applicable identical or different, radicals  $R_{18}$ ;

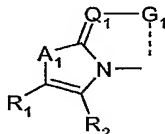
- 60 -

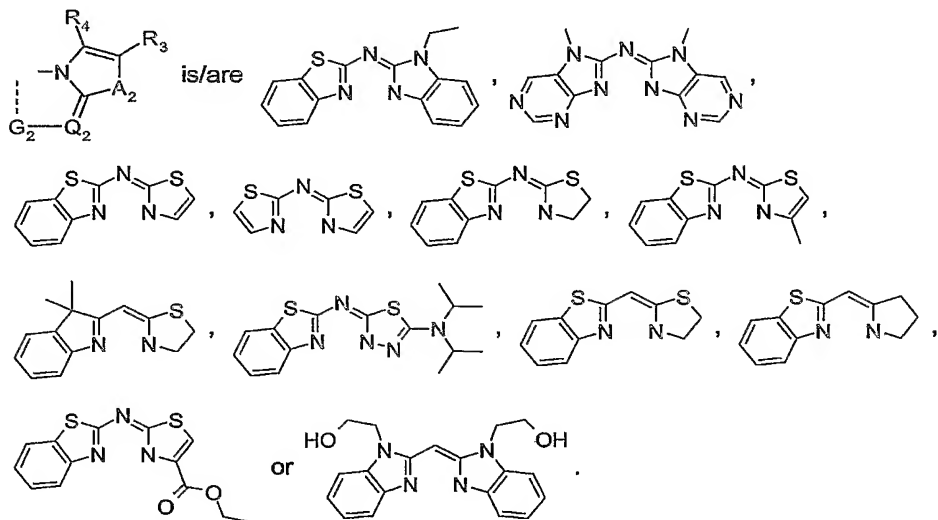
R<sub>15</sub> is hydrogen, cyano, COO-R<sub>25</sub> or C<sub>1</sub>-C<sub>12</sub>alkyl;

R<sub>17</sub> is halogen, hydroxy, O-R<sub>25</sub>, cyano, COO-R<sub>25</sub> or carboxy; and

R<sub>18</sub> is halogen, nitro, cyano, O-R<sub>19</sub>, CH=C(CN)<sub>2</sub>, COOR<sub>19</sub>, ureido, CONR<sub>25</sub>R<sub>26</sub>, SO<sub>2</sub>R<sub>25</sub>, P(=O)OR<sub>19</sub>OR<sub>23</sub> or unsubstituted or substituted C<sub>1</sub>-C<sub>12</sub>alkyl.

- 5 3. An optical recording medium according to claim 1 or 2, wherein the recording

layer comprises a compound of formula (I) wherein  and/or



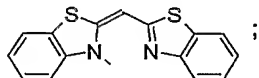
4. An optical recording medium according to claim 1, 2 or 3, wherein the compound of formula (I) contains branched C<sub>3</sub>-C<sub>24</sub>alkyl or branched C<sub>3</sub>-C<sub>24</sub>alkenyl.

5. An optical recording medium according to claim 1, 2, 3 or 4, wherein the recording layer is substantially amorphous.

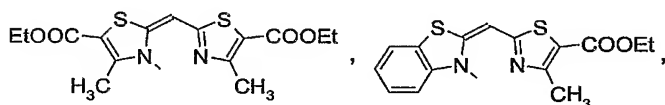
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6. An optical recording medium according to claim 1, 2, 3, 4 or 5, additionally comprising a covering layer, wherein substrate, reflector layer, recording layer and covering layer are arranged in that order.
7. An optical recording medium according to claim 1, 2, 3, 4, 5 or 6, which in addition to comprising a compound of formula (I) comprises a metal-free chromophore.
8. A method of recording or playing back data, wherein the data on an optical recording medium according to claim 1, 2, 3, 4, 5, 6 or 7 are recorded or played back at a wavelength of from 350 to 500 nm.
9. A compound of formula (I) according to claim 1, with the proviso that the compound is not a compound of formula  $M_2(Z_1)_2$ , wherein:

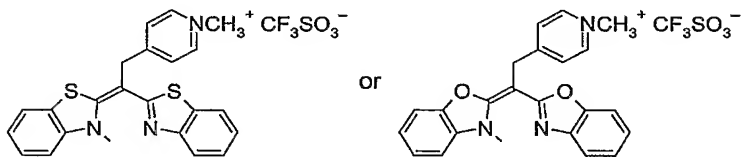
- $M_2$  is Co(II), Cu(II), Hg(II), Ni(II), Pd(II) or Zn(II) and  $Z_1$  is



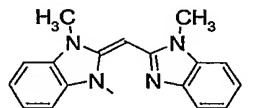
- $M_2$  is Co(II), Cu(II), Ni(II), Pd(II) or Zn(II) and  $Z_1$  is



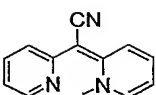
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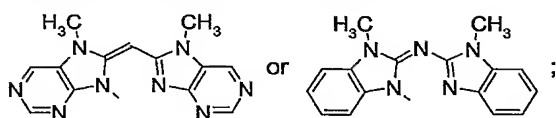
- $M_2$  is Co(II), Cu(II), Ni(II) or Zn(II) and  $Z_1$  is



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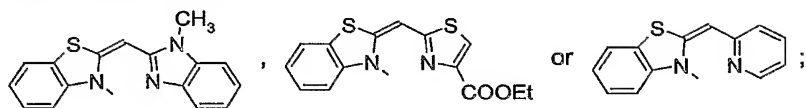
- $M_2$  is Cu(II), Pd(II) or Zn(II) and  $Z_1$  is  ;

- $M_2$  is Co(II), Cu(II) or Zn(II) and  $Z_1$  is

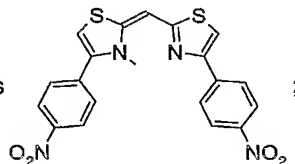


- $M_2$  is Cu(II) or Zn(II) and  $Z_1$  is

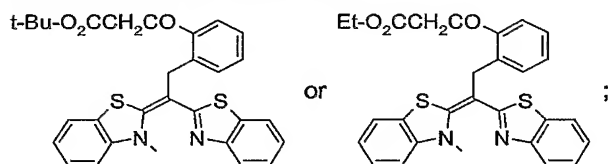
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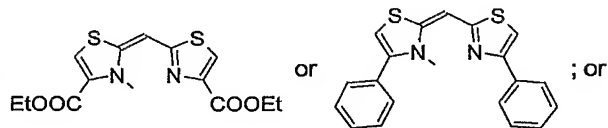
- $M_2$  is Co(II) or Cu(II) and  $Z_1$  is



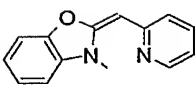
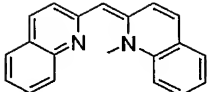
- $M_2$  is Pd(II) or Zn(II) and  $Z_1$  is



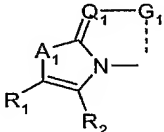
- $M_2$  is Cu(II) and  $Z_1$  is

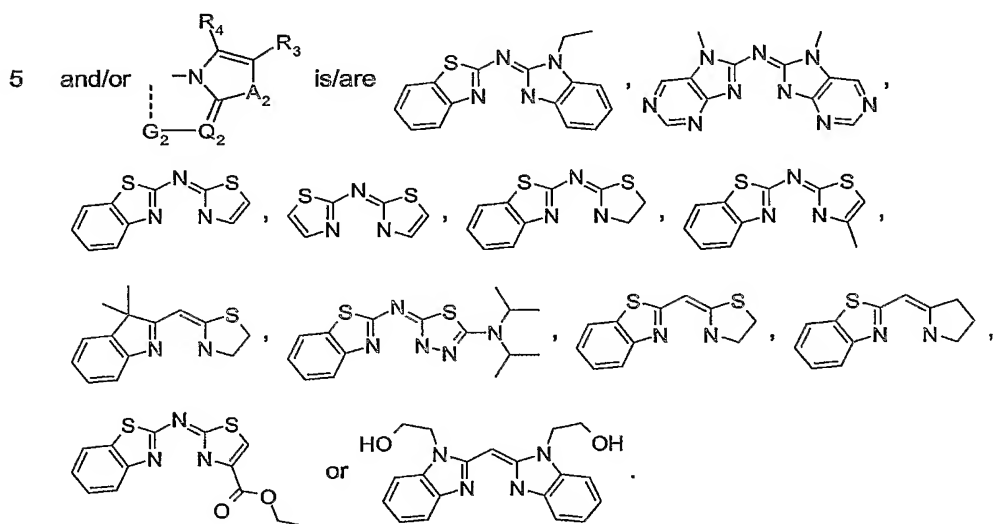


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- $M_2$  is Zn(II) and  $Z_1$  is  or .

10. A compound according to claim 9, containing branched  $C_3$ - $C_{24}$ alkyl or branched  $C_3$ - $C_{24}$ alkenyl.

11. A compound according to claim 9 or 10 of formula (I), wherein 





# INTERNATIONAL SEARCH REPORT

International Application No  
PCT/EP2004/050185

**A. CLASSIFICATION OF SUBJECT MATTER**  
IPC 7 G11B7/24 C07D403/02

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)  
IPC 7 G11B C07D

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data, PAJ, CHEM ABS Data

## C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	EP 1 130 584 A (MITSUI CHEMICAL) 5 September 2001 (2001-09-05) claim 1	1,8,9
A	US 5 962 657 A (H WOLLEB) 5 October 1999 (1999-10-05) column 3, line 28 - column 6, line 41; claim 1	1,8,9
A	DE 19 32 894 A (BASF) 28 January 1971 (1971-01-28) claim 1	9
A	US 6 376 664 B1 (M K CHAN) 23 April 2002 (2002-04-23) claims 1,2	9

☐ Further documents are listed in the continuation of box C.

☒ Patent family members are listed in annex.

### \* Special categories of cited documents :

- \*A\* document defining the general state of the art which is not considered to be of particular relevance
- \*E\* earlier document but published on or after the international filing date
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- \*O\* document referring to an oral disclosure, use, exhibition or other means
- \*P\* document published prior to the international filing date but later than the priority date claimed

- \*T\* later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
- \*X\* document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
- \*Y\* document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.
- \* & \* document member of the same patent family

Date of the actual completion of the international search

12 July 2004

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21/07/2004

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Authorized officer

Vanhecke, H

# INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No  
PCT/EP2004/050185

Patent document cited in search report		Publication date	Patent family member(s)	Publication date
EP 1130584	A	05-09-2001	CN 1317789 A	17-10-2001
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			JP 2002212456 A	31-07-2002
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**DERWENT-ACC-NO:** 2004-728406**DERWENT-WEEK:** 200735*COPYRIGHT 2007 DERWENT INFORMATION LTD*

**TITLE:** Optical recording medium, e.g. compact disc for computer, includes recording layer comprising (new) transition metal complex of nitrogen-containing heterocyclic ligand

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BUDRY, J L

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CHEM HOLDING INC[CIBA] , CIBA SPECIALTY CHEM  
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[SUTTI]

**PRIORITY-DATA:** 2003CH-0000331 (March 3, 2003)

**PATENT-FAMILY:**

<b>PUB-NO</b>	<b>PUB-DATE</b>	<b>LANGUAGE</b>	<b>PAGES</b>	<b>MAIN-IPC</b>
IN 200502505 P4	March 30, 2007	E	000	G11B 007/24
WO 2004079732 A1	September 16, 2004	E	066	G11B 007/24
EP 1599878 A1	November 30, 2005	E	000	G11B 007/24
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DE 6004001135 T2	April 12, 2007	N/A	000	G11B 007/24

**DESIGNATED-STATES:** AE AG AL AM AT AU AZ BA BB BG BR BW BY BZ CA  
 CH CN CO CR CU CZ DE DK DM DZ EC EE EG ES FI  
 GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP  
 KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW  
 MX MZ NA NI NO NZ OM PG PH PL P T RO RU SC  
 SD SE SG SK SL SY TJ TM TN TR TT TZ UA UG US  
 UZ VC VN YU ZA ZM ZW AT BE BG BW CH CY CZ DE  
 DK EA EE ES FI FR GB GH GM GR HU IE IT KE LS  
 LU MC MW MZ NL OA PT RO SD SE SI SK SL SZ TR  
 TZ UG ZM ZW AL AT BE BG CH CY CZ DE DK EE ES  
 FI FR GB GR HU IE I T LI LT LU LV MC MK NL  
 PT RO SE SI SK TR AT BE BG CH CY CZ DE DK EE  
 ES FI FR GB GR HU IE IT LI LU MC NL PT RO SE  
 SI SK TR

**APPLICATION-DATA:**

<b>PUB-NO</b>	<b>APPL-DESCRIPTOR</b>	<b>APPL-NO</b>	<b>APPL-DATE</b>
IN 200502505P4	N/A	2004WO-EP50185	February 23, 2004
IN 200502505P4	N/A	2005IN-CN02505	October 3, 2005
WO2004079732A1	N/A	2004WO-EP50185	February 23, 2004
EP 1599878A1	N/A	2004EP-0713552	February 23, 2004
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EP 1599878A1	Based on	WO2004079732	N/A
TW 200428381A	N/A	2004TW-0105419	March 2, 2004
EP 1599878B1	N/A	2004EP-0713552	February 23, 2004
EP 1599878B1	N/A	2004WO-EP50185	February 23, 2004
EP 1599878B1	Based on	WO2004079732	N/A
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DE6004001135E	N/A	2004WO-EP50185	February 23, 2004
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KR2005115265A	N/A	2004WO-EP50185	February 23, 2004
KR2005115265A	N/A	2005KR-0716423	September 2, 2005
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DE6004001135T2	Based on	EP 1599878	N/A
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**INT-CL (IPC):** B32B003/02, B41M005/26 , C07D403/00 ,  
C07D403/02 , C07F001/08 , C07F015/04 ,  
C07F015/06 , C09B023/00 , C09B055/00 ,  
C09B057/00 , C09B057/10 , G11B007/24 ,  
G11B007/244

**RELATED-ACC-NO:** 2005-664282

**ABSTRACTED-PUB-NO:** WO2004079732A

**BASIC-ABSTRACT:**

NOVELTY - An optical recording medium comprises a substrate, a recording layer and optionally reflecting layer(s). The

recording layer comprises transition metal complex (I) of nitrogen-containing heterocyclic ligand, or its tautomer, some of which are new.

DETAILED DESCRIPTION - An optical recording medium comprises a substrate, a recording layer and optionally reflecting layer(s). The recording layer comprises a complex of formula (I) or its tautomer.

G1, G2 = a group of structures (IX)-(XII);

A1, A2 = N(R12), O, S or Se;

A3 = C(1-5C alkyl)2, C(4-5C alkylene), N(R12), O, S, Se, N=C(R13) or unsubstituted or R14-substituted CH=CH;

M1 = transition metal of groups IX-XII, preferably Co, Cu, Ni, Pd or Zn;

Q1, Q2 = C(R15), N or P;

R1-R8, R14 = H, R18, 6-12C aryl, 4-12C heteroaryl, 7-12C aralkyl or 5-12C heteroaralkyl, each optionally substituted by radicals R18;

R9, R12, R13 = 1-24C alkyl, 3-24C cycloalkyl, 2-24C alkenyl, 3-24C cycloalkenyl, 1-4C alkyl-(O-1-4C alkylene)O-1-4C alkylene)m or 1-4C alkyl-(NH-1-4C alkylene)m, each of which substituted by radicals R17; or 6-12C aryl, 4-12C heteroaryl, 7-12C aralkyl or 5-12C heteroaralkyl, each optionally substituted by radicals R18;

R10, R11, R18 = halo, nitro, cyano, thiocyno, hydroxy, O-R19, O-CO-R19, S-R19, CHO, COR20, CHOR19OR23, CR20OR19OR23, R16, N=N-R16, N=CR19R20, N=CR21R22, C(R15)=NR19, C(R15)=NR21, C(R15)=CR21R22, NH2, NH-R19, NR19R20, N=CR21R22, C(R15)=NR19, C(R15)=NR21, C(R15)=NR21R22, NH2, NH-R19, NR19R21, NH3+, NH2R19+, NHR19R20+, NR19R20R23+, CONH2, CONHR19, CONR19R20, SO2R19, SO2NH2, SO2NHR19, SO2NR19R20, COOH, COOR19, OCOOR19, NHCOR19, NR19COR23, NHCOOR19, NR19COOR23, ureido, NR19-CO-NHR23, B(OH)2, B(OH)(OR19), B(OR19)OR23, phosphato, PR19R23, POR19OR23, P(=O)OR19OR23, OPR19R23, OPR19OR23, OP(=O)R19OR23, OP(=O)OR19OR23, OPO3R19, sulfato, sulfo or 1-12C alkyl, 3-12C cycloalkyl, 1-12C alkylthio, 3-12C cycloalkylthio, 3-12C alkoxy or 3-12C cycloalkoxy, each optionally substituted by radicals R17;

R15 = H, cyano, hydroxy, 1-12C alkoxy, 3-12C cycloalkoxy, 1-12C alkylthio, 3-12C cycloalkylthio, amino, NHR24, NR25R26, R27, halo, nitro, formyl, N=N-R27, C(R14)=CR21R22, C(R14)=NR19, COO-R25, carboxy, carbamoyl, CONH-R25, CONR25R26, N=CR19R20, or 1-12C alkyl, 3-12C cycloalkyl, 2-12C alkenyl or 3-12C cycloalkenyl each optionally substituted by halo, hydroxy, 1-12C alkoxy or 3-12C cycloalkoxy;

R16 = 6-12C aryl, 4-12C heteroaryl, 7-12C aralkyl or 5-12C heteroaralkyl, each optionally substituted by radical R29;

R17 = halo, hydroxy, O-R25, O-CO-R25, S-R25, NH2, NH-R25, NR25R26, NH3+, NH2R25+, NHR25R26+, NR24R25R26+, NR25-CO-R24, NR25COOR24, cyano, formyl, COO-R25, carboxy, carbamoyl, CONH-R25, CONR25R26, ureido, NH-CO-NHR24, NR25-CO-NHR24, phosphato, PR25R24, POR25OR24, P(=O)OR25OR24, OPR25R24, OPR25OR24, OP(=O)R25OR24, OP(=O)OR25OR24, SO2R25, sulfato, sulfo, R27, N=N-R27 or 1-12C alkoxy or 1-12C cycloalkoxy each unsubstituted or mono- or poly-substituted by halo;

R19, R20, R23 = R16, or 1-12C alkyl, 3-12C cycloalkyl, 2-12C alkenyl, or 3-12C cycloalkenyl, each optionally substituted by halo, hydroxy, 1-12C alkoxy or 3-12C cycloalkoxy;

R21, R22 = NR25R26, CN, CONH2, CONHR19, CONR19R20 or COOR20;

R24-R26 = 1-12C alkyl, 3-12C cycloalkyl, 2-12C alkenyl, 3-12C cycloalkenyl, 6-12C aryl, 4-12C heteroaryl, 7-12C aralkyl or 5-12C heteroaralkyl;

R27 = 6-12C alkyl, 4-12C heteroalkyl, 7-12C aralkyl, or 5-12C heteroaralkyl, each optionally substituted by radicals R18;

R28 = nitro, SO2NHR25, SO2NR25R26, 1-12C alkyl, 3-12C cycloalkyl, 1-12C alkylthio, 3-12C cycloalkylthio, 1-12C alkoxy or 3-12C cycloalkoxy, each optionally substituted by radicals R17;

m = 1-10.

Optionally, R1+R2, R3+R4, R5+R6, R5+R13 and/or R5+R14 together in pairs are 3-6C alkylene or 3-6C alkenylene, each of which is optionally substituted by radicals R17 and may be interrupted by O, S or N(R12), or 1,4-buta-1,3-dienylene, groups of structure (1) or (2), each optionally substituted by radical R18 and in which 1 or 2 carbon atoms may have been replaced by nitrogen. R14

+R19, R15+R19 and/or R19+R23 together are 3-12C cycloalkyl, 2-12C alkenyl or 3-12C cycloalkenyl, each optionally substituted by halo, hydroxy, 1-12C alkoxy or 3-12C cycloalkoxy. R19+R20 together with the common nitrogen are pyrrolidine, piperidine, piperazine, or morpholine, each unsubstituted or mono- to tetra-substituted by 1-4C alkyl; or cabazole, phenoxazine or phenothiazine, each optionally substituted by radicals R28. R25+R26 together with the common nitrogen are pyrrolidine, piperidine, piperazine or morpholine, each unsubstituted, or mono- to tetra-substituted by 1-4C alkyl.

INDEPENDENT CLAIMS are also included for:

(1) a method of recording or playing back data comprising recording or playing back the data on the optical recording medium at a wavelength of 350-500 nm; and

(2) new compounds (I) with the exception of those disclosed in J. Org. Chem. 67/16 5753-5772 (2002).

The new (I) are not e.g. compounds of formula  $M_2(Z_1)_2$  where  $M_2$  is Co(II), Cu(II), Hg(II), Ni(II), Pd(II) or Zn(II) and  $Z_1$  is a group of formula (a).

or where  $M_2$  is Co(II), Cu(II), Ni(II), Pd(II) or Zn(II) and  $Z_1$  is a group of formula (b)-(f).

Many other combinations of excluded metals and ligands are specified.

USE - The recording medium, e.g. compact disc or digital video disc, is used in computers and as storage material for identification and security cards or for the production of optical elements, e.g. holograms.

ADVANTAGE - The optical recording materials have excellent recording and playback quality especially at a wavelength of 350-500 nm. Recording and playback can be effected very advantageously with high sensitivity at the same wavelength, and the storage density is higher than in the case of known materials. The materials have very good storage properties before and after recording, even under especially harsh conditions, e.g. exposure to sunlight or fluorescent lighting, heat and/or high humidity. The manufacture is simple and readily reproducible using customary coating processes, e.g. spin-coating. The optical recording medium has high information



density, sensitivity and data reliability. It is robust, durable and easy to use. It is inexpensive to manufacture.

**CHOSEN-DRAWING:** Dwg.0/0

**TITLE-TERMS:** OPTICAL RECORD MEDIUM COMPACT DISC COMPUTER  
RECORD LAYER COMPRISE NEW TRANSITION METAL  
COMPLEX NITROGEN CONTAIN HETEROCYCLE LIGAND

**DERWENT-CLASS:** E12 L03 P73 P75 T03

**CPI-CODES:** E05-L; E05-M; E05-N; L03-G04B;

**EPI-CODES:** T03-B01B1; T03-B01D1; T03-B01D3;

**CHEMICAL-CODES:** Chemical Indexing M3 \*01\* Fragmentation Code  
A429 A960 C710 D012 D019 D022 D029 E600 E699 K0  
L3 L355 L9 L922 L999 M1 M126 M143 M210 M211  
M240 M282 M320 M411 M512 M520 M530 M540 M630  
M781 M904 M905 Q454 R043 Specfic Compounds  
AFHU8K AFHU8U

Chemical Indexing M3 \*02\* Fragmentation Code  
A429 A960 C710 D012 D019 E600 E699 K0 L3 L355  
L9 L922 L999 M1 M126 M143 M280 M320 M411 M512  
M520 M530 M540 M630 M781 M904 M905 Q454 R043  
Specfic Compounds AFHUAK AFHUAU

Chemical Indexing M3 \*03\* Fragmentation Code  
A429 A960 C710 D012 D019 D022 D029 E400 E499 H7  
H720 M1 M126 M132 M210 M214 M233 M240 M282 M311  
M321 M343 M411 M512 M520 M530 M540 M630 M781  
M904 M905 Q454 R043 Specfic Compounds AFHUCK  
AFHUCU

Chemical Indexing M3 \*04\* Fragmentation Code  
A428 A960 C710 D012 D019 D022 D029 E600 E699 H5  
H542 H8 K0 L3 L355 L9 L922 L999 M1 M126 M143  
M210 M211 M272 M282 M320 M411 M512 M520 M530  
M540 M630 M781 M904 M905 Q454 R043 Specfic  
Compounds AFHULK AFHULU

Chemical Indexing M3 \*05\* Fragmentation Code  
A429 A960 C710 D012 D019 D022 D029 E600 E699 H5  
H542 H8 K0 L3 L355 L9 L922 L999 M1 M126 M143  
M210 M211 M272 M282 M320 M411 M512 M520 M530  
M540 M630 M781 M904 M905 Q454 R043 Specfic  
Compounds AFHUNK AFHUNU

Chemical Indexing M3 \*06\* Fragmentation Code  
A429 A960 C316 C710 D012 D019 D022 D029 E600  
E699 H7 H720 K0 K4 K442 K499 M1 M126 M132 M210  
M212 M271 M282 M311 M321 M343 M411 M512 M520  
M530 M540 M630 M781 M904 M905 Q454 R043 Specfic  
Compounds AFHURK AFHURU

Chemical Indexing M3 \*07\* Fragmentation Code  
A427 A960 C710 D012 D019 D022 D029 E600 E699 K0  
L3 L355 L9 L922 L999 M1 M126 M143 M210 M211  
M240 M282 M320 M411 M512 M520 M530 M540 M630  
M781 M904 M905 Q454 R043 Specfic Compounds  
AFHUTK AFHUTU

Chemical Indexing M3 \*08\* Fragmentation Code  
A427 A960 C710 D012 D019 D022 D029 E600 E699 H5  
H542 H8 K0 L3 L355 L9 L922 L999 M1 M126 M143  
M210 M211 M272 M282 M320 M411 M512 M520 M530  
M540 M630 M781 M904 M905 Q454 R043 Specfic  
Compounds AFHUXK AFHUXU

Chemical Indexing M3 \*09\* Fragmentation Code  
A428 A960 C710 D012 D019 D022 D029 E600 E699 K0  
L3 L355 L9 L922 L999 M1 M126 M143 M210 M211  
M240 M282 M320 M411 M512 M520 M530 M540 M630  
M781 M904 M905 Q454 R043 Specfic Compounds  
AFHV0K AFHV0U

Chemical Indexing M3 \*10\* Fragmentation Code  
A428 A960 C316 C710 D012 D019 D022 D029 E400  
E499 H7 H720 K0 K4 K442 K499 M1 M126 M132 M210  
M212 M271 M282 M311 M321 M343 M411 M512 M520  
M530 M540 M630 M781 M904 M905 Q454 R043 Specfic  
Compounds AFHV1K AFHV1U

Chemical Indexing M3 \*11\* Fragmentation Code  
A427 A960 C710 F012 F014 F019 F710 F799 K0 L3  
L355 L9 L922 L999 M1 M126 M143 M210 M211 M240  
M282 M320 M411 M510 M522 M530 M540 M630 M781  
M904 M905 Q454 R043 Specfic Compounds AFHV9K  
AFHV9U

Chemical Indexing M3 \*12\* Fragmentation Code  
A428 A960 C710 D012 D019 D022 D029 E600 E699 K0  
L3 L355 L9 L922 L999 M1 M126 M143 M210 M214

M233 M240 M282 M320 M411 M512 M520 M530 M540  
M630 M781 M904 M905 Q454 R043 Specfic Compounds  
AFHVBK AFHVBV

Chemical Indexing M3 \*13\* Fragmentation Code  
A429 A960 C710 D012 D019 D022 D029 E600 E699 K0  
L3 L355 L9 L922 L999 M1 M126 M143 M210 M214  
M233 M240 M282 M320 M411 M512 M520 M530 M540  
M630 M781 M904 M905 Q454 R043 Specfic Compounds  
AFHVDK AFHVDU

Chemical Indexing M3 \*14\* Fragmentation Code  
A427 A960 C710 D012 D019 D022 D029 E600 E699 K0  
L3 L355 L9 L922 L999 M1 M126 M143 M210 M214  
M233 M240 M282 M320 M411 M512 M520 M530 M540  
M630 M781 M904 M905 Q454 R043 Specfic Compounds  
AFHVLK AFHVLU

Chemical Indexing M3 \*15\* Fragmentation Code  
A428 A960 C710 F012 F014 F019 F710 F799 K0 L3  
L355 L9 L922 L999 M1 M126 M143 M210 M211 M240  
M282 M320 M411 M510 M522 M530 M540 M630 M781  
M904 M905 Q454 R043 Specfic Compounds AFHVNK  
AFHVNU

Chemical Indexing M3 \*16\* Fragmentation Code  
A427 A960 C710 D012 D019 D022 D029 E400 E499 H7  
H720 M1 M126 M132 M210 M214 M233 M240 M282 M311  
M321 M343 M411 M512 M520 M530 M540 M630 M781  
M904 M905 Q454 R043 Specfic Compounds AFHVPK  
AFHVPU

Chemical Indexing M3 \*17\* Fragmentation Code  
A429 A960 C710 F012 F014 F019 F710 F799 K0 L3  
L355 L9 L922 L999 M1 M126 M143 M210 M211 M240  
M281 M320 M411 M510 M522 M530 M540 M630 M781  
M904 M905 Q454 R043 Specfic Compounds AFHVKW  
AFHVVU

Chemical Indexing M3 \*18\* Fragmentation Code  
A428 A960 C710 F012 F014 F019 F710 F799 K0 L3  
L355 L9 L922 L999 M1 M126 M143 M210 M211 M240  
M281 M320 M411 M510 M522 M530 M540 M630 M781  
M904 M905 Q454 R043 Specfic Compounds AFHW1K  
AFHW1U

Chemical Indexing M3 \*19\* Fragmentation Code  
A427 A960 C710 F012 F014 F019 F710 F799 K0 L3  
L355 L9 L922 L999 M1 M126 M143 M210 M211 M240  
M281 M320 M411 M510 M522 M530 M540 M630 M781  
M904 M905 Q454 R043 Specfic Compounds AFHW6K  
AFHW6U

Chemical Indexing M3 \*20\* Fragmentation Code  
A428 A960 C710 D012 D019 E400 E499 H7 H720 M1  
M126 M132 M280 M311 M321 M343 M411 M512 M520  
M530 M540 M630 M781 M904 M905 Q454 R043 Specfic  
Compounds AFHW8K AFHW8U

Chemical Indexing M3 \*21\* Fragmentation Code  
A428 A960 C710 D012 D019 D022 D029 E400 E499 H7  
H720 M1 M126 M132 M210 M214 M233 M240 M282 M311  
M321 M343 M411 M512 M520 M530 M540 M630 M781  
M904 M905 Q454 R043 Specfic Compounds AFHW9K  
AFHW9U

Chemical Indexing M3 \*22\* Fragmentation Code  
A427 A960 C710 D012 D019 E400 E499 H7 H720 M1  
M126 M132 M280 M311 M321 M343 M411 M512 M520  
M530 M540 M630 M781 M904 M905 Q454 R043 Specfic  
Compounds AFHWCK AFHWCU

Chemical Indexing M3 \*23\* Fragmentation Code  
A427 A960 C710 D012 D019 E600 E699 K0 L3 L355  
L9 L922 L999 M1 M126 M143 M280 M320 M411 M512  
M520 M530 M540 M630 M781 M904 M905 Q454 R043  
Specfic Compounds AFHWDK AFHWDU

Chemical Indexing M3 \*24\* Fragmentation Code  
A428 A960 C710 D012 D019 E600 E699 K0 L3 L355  
L9 L922 L999 M1 M126 M143 M280 M320 M411 M512  
M520 M530 M540 M630 M781 M904 M905 Q454 R043  
Specfic Compounds AFHWFK AFHWFU

Chemical Indexing M3 \*25\* Fragmentation Code  
A429 A960 C710 D012 D019 E400 E499 H7 H720 M1  
M126 M132 M280 M311 M321 M343 M411 M512 M520  
M530 M540 M630 M781 M904 M905 Q454 R043 Specfic  
Compounds AFHWGK AFHWGU

Chemical Indexing M3 \*26\* Fragmentation Code  
A428 A960 C710 D012 D019 E400 E499 H7 H720 M1

M126 M132 M280 M312 M321 M331 M340 M343 M411  
M512 M520 M530 M540 M630 M781 M904 M905 Q454  
R043 Specfic Compounds AFHWHK AFHWHU

Chemical Indexing M3 \*27\* Fragmentation Code  
A427 A960 C710 D012 D019 E400 E499 H7 H720 M1  
M126 M132 M280 M312 M321 M331 M340 M343 M411  
M512 M520 M530 M540 M630 M781 M904 M905 Q454  
R043 Specfic Compounds AFHWWK AFHWWU

Chemical Indexing M3 \*28\* Fragmentation Code  
A429 A960 C710 D012 D019 E400 E499 H7 H720 M1  
M126 M132 M280 M312 M321 M331 M340 M343 M411  
M512 M520 M530 M540 M630 M781 M904 M905 Q454  
R043 Specfic Compounds AFHWLK AFHWLU

Chemical Indexing M3 \*29\* Fragmentation Code  
A429 A960 C710 F012 F014 F019 F710 F799 K0 L3  
L355 L9 L922 L999 M1 M126 M143 M210 M211 M240  
M282 M320 M411 M510 M522 M530 M540 M630 M781  
M904 M905 Q454 R043 Specfic Compounds AFHWMK  
AFHWMU

Chemical Indexing M3 \*30\* Fragmentation Code  
A428 A960 C710 F012 F015 F019 F710 F799 K0 L3  
L355 L9 L922 L999 M1 M126 M143 M210 M211 M240  
M282 M320 M411 M510 M522 M530 M540 M630 M781  
M904 M905 Q454 R043 Specfic Compounds AFHWNK  
AFHWNLU

Chemical Indexing M3 \*31\* Fragmentation Code  
A427 A960 C710 F012 F015 F019 F710 F799 K0 L3  
L355 L9 L922 L999 M1 M126 M143 M210 M211 M240  
M282 M320 M411 M510 M522 M530 M540 M630 M781  
M904 M905 Q454 R043 Specfic Compounds AFHWOK  
AFHWOU

Chemical Indexing M3 \*32\* Fragmentation Code  
A429 A960 C710 F012 F015 F019 F710 F799 K0 L3  
L355 L9 L922 L999 M1 M126 M143 M210 M211 M240  
M282 M320 M411 M510 M522 M530 M540 M630 M781  
M904 M905 Q454 R043 Specfic Compounds AFHWPK  
AFHWPU

Chemical Indexing M3 \*33\* Fragmentation Code  
A427 A428 A429 A430 A546 A960 B605 B615 B634

B701 B702 B712 B713 B720 B740 B741 B742 B743  
B744 B803 B813 B815 B831 B832 B833 B834 C710  
D013 D021 D022 D023 D700 F011 F012 F013 F014  
F015 F016 F017 F019 F020 F022 F029 F421 F422  
F423 F431 F432 F511 F512 F521 F522 F523 F530  
F541 F542 F570 F580 F599 F610 F630 F699 F710  
F730 F799 G001 G002 G010 G011 G012 G013 G019  
G020 G021 G022 G029 G030 G031 G032 G039 G040  
G050 G051 G052 G100 G111 G112 G113 G221 G299  
G553 G563 H100 H101 H103 H121 H122 H123 H161  
H162 H181 H182 H201 H202 H211 H321 H322 H323  
H401 H402 H403 H404 H405 H421 H422 H423 H424  
H521 H522 H523 H592 H599 H600 H607 H608 H609  
H621 H622 H623 H721 J011 J012 J013 J014 J111  
J112 J113 J211 J212 J221 J222 J311 J312 J411  
J412 J581 J582 J583 K421 K431 K499 K534 K599  
L120 L142 L199 L355 L399 L472 L499 L640 L650  
L660 L699 L722 L724 L910 L921 L922 L941 L943  
L999 M1 M113 M115 M116 M119 M123 M125 M126 M129  
M132 M135 M139 M141 M142 M143 M144 M149 M150  
M210 M211 M212 M213 M214 M215 M216 M220 M221  
M222 M223 M224 M225 M226 M231 M232 M233 M240  
M262 M263 M271 M272 M273 M280 M281 M282 M283  
M311 M312 M313 M314 M315 M316 M320 M321 M322  
M323 M331 M332 M333 M340 M342 M343 M373 M391  
M392 M393 M411 M510 M511 M521 M522 M523 M530  
M531 M532 M533 M540 M541 M542 M543 M630 M781  
M904 M905 Q454 R043 Ring Index 00085 00090  
00093 00096 00123 00211 00995 01218 01293 41935  
Markush Compounds 200140-51401-K 200140-51401-U

**SECONDARY-ACC-NO:****CPI Secondary Accession Numbers:** C2004-255905**Non-CPI Secondary Accession Numbers:** N2004-576927